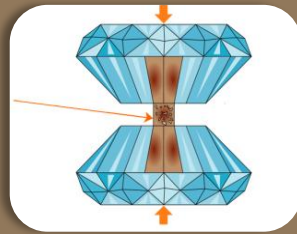


TOPOLOGICAL STUDY OF CHEMICAL BONDS UNDER PRESSURE: Hydrogen as a model case



Vanessa Labet
Paris, FRANCE



Neil
ASHCROFT



Roald
HOFFMANN

Postdoc 2009-2011

Cornell Univ.





Neil
ASHCROFT



Roald
HOFFMANN

Postdoc 2009-2011

Cornell Univ.

Univ. P. & M. Curie

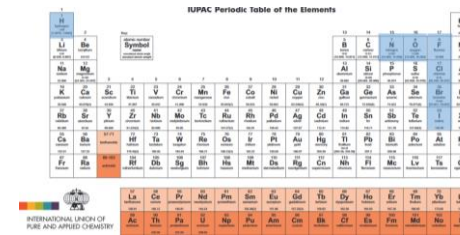


Vanessa
RIFFET



Julia
CONTRERAS
-GARCIA

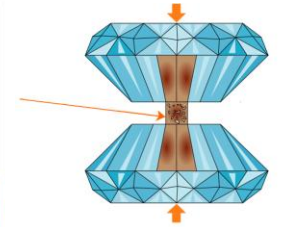
1. Intro - **Molecular solids** under pressure: generalities
2. Solid Hydrogen under pressure : focus on the H---H distances (intra + intermolecular) - *Cornell*
3. Study of a non periodic model for solid H under pressure : topological tools (NCI + ELF)



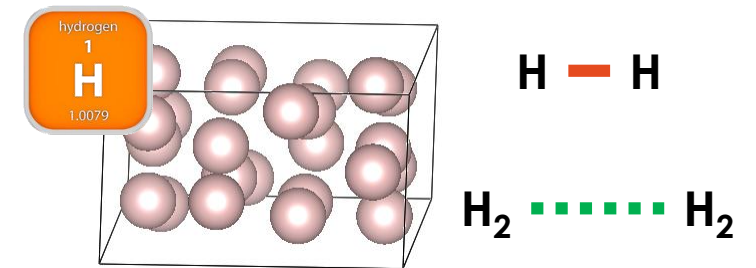
IUPAC Periodic Table of the Elements

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

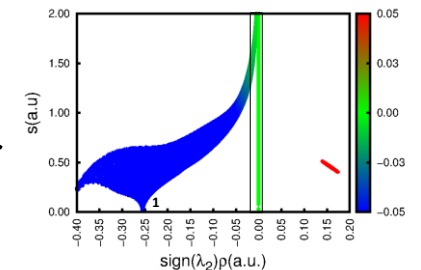
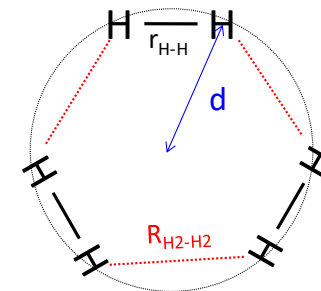
The image shows a standard periodic table of elements with color-coded groups. The lanthanide and actinide series are shown in separate rows below the main table. The logo of the International Union of Pure and Applied Chemistry (IUPAC) is visible at the bottom left of the table.



1. Intro - **Molecular solids** under pressure: generalities
2. Solid **Hydrogen** under pressure : focus on the **H---H distances** (intra + intermolecular) - *Cornell*
3. Study of a non periodic model for solid H under pressure : topological tools (NCI + ELF)



1. Intro - **Molecular solids** under pressure: generalities
2. Solid **Hydrogen** under pressure : focus on the **H---H distances** (intra + intermolecular) - *Cornell*
3. Study of a **non periodic model** for solid H under pressure : **topological tools** (NCI + ELF)



Reviews

W. Grochala et al.

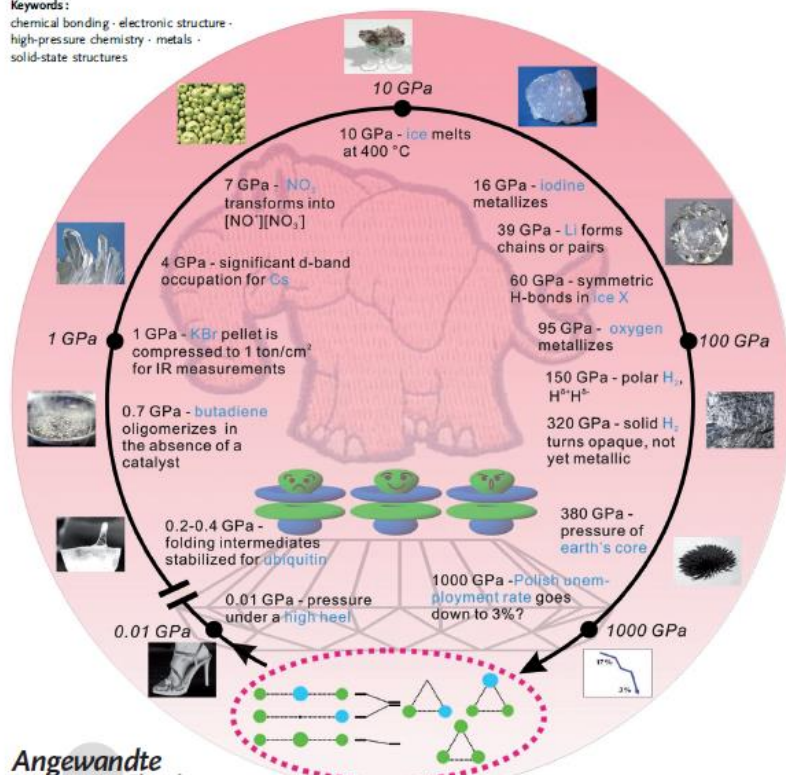
High-Pressure Chemistry

DOI: 10.1002/anie.200602485

The Chemical Imagination at Work in *Very Tight Places*

Wojciech Grochala,* Roald Hoffmann,* Ji Feng,* and Neil W. Ashcroft*

Keywords:
chemical bonding · electronic structure ·
high-pressure chemistry · metals ·
solid-state structures



Angewandte

Grochala et al. Angew. Chem. Int. Ed. 2007, 46, 3620-3642

Molecular solids under Pressure :

$$T = 0K \quad \text{Enthalpy} \quad H = E + pV$$

Finding ways of decreasing volume V

1. Squeezing the « van der Waals space »
2. Increasing coordination numbers
3. Shortening bonds
4. Electrons moving off their atoms

IUPAC Periodic Table of the Elements

1 H hydrogen 1.008 [1.0078, 1.0082]																	18 He helium 4.0026
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.808, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]											13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.088]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.798(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Key:
atomic number
Symbol
name
conventional atomic weight
standard atomic weight

Molecular solids under Pressure :

1. Squeezing the « van der Waals space »
2. Increasing coordination numbers
3. Shortening bonds
4. Electrons moving off their atoms

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

For notes and updates to this table, see www.iupac.org. This version is dated 28 November 2016.
Copyright © 2016 IUPAC, the International Union of Pure and Applied Chemistry.

IUPAC Periodic Table of the Elements

1 H hydrogen 1.008 [1.0078, 1.0082]																	18 He helium 4.0026
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.808, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]											13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.088]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.798(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium 98	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium 209	85 At astatine 210	86 Rn radon 222
87 Fr francium 223	88 Ra radium 226	89-103 actinoids	104 Rf rutherfordium 261	105 Db dubnium 262	106 Sg seaborgium 263	107 Bh bohrium 264	108 Hs hassium 265	109 Mt meitnerium 266	110 Ds darmstadtium 267	111 Rg roentgenium 268	112 Cn copernicium 269	113 Nh nihonium 270	114 Fl flerovium 271	115 Mc moscovium 272	116 Lv livermorium 273	117 Ts tennessine 274	118 Og oganesson 275

Key:
atomic number
Symbol
name
conventional atomic weight
standard atomic weight

Molecular solids under Pressure :

1. Squeezing the « van der Waals space »
2. Increasing coordination numbers
3. Shortening bonds
4. Electrons moving off their atoms

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium 145	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium 227	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium 237	94 Pu plutonium 244	95 Am americium 243	96 Cm curium 247	97 Bk berkelium 247	98 Cf californium 251	99 Es einsteinium 252	100 Fm fermium 257	101 Md mendelevium 258	102 No nobelium 259	103 Lr lawrencium 260

For notes and updates to this table, see www.iupac.org. This version is dated 28 November 2016.
Copyright © 2016 IUPAC, the International Union of Pure and Applied Chemistry.

IUPAC Periodic Table of the Elements

Key: atomic number, Symbol, name

NITROGEN

$P = 1 \text{ atm}$ $P = 115 \text{ GPa}$

$\alpha\text{-N}_2$ (molecular) Cubic gauche N (monatomic)

CN = 1 ($d_{\text{N-N}} = 106 \text{ pm}$) CN = 3 ($d_{\text{N-N}} = 146 \text{ pm}$)

- single : $d_{\text{N-N}} = 142 \text{ pm}$
- double: $d_{\text{N-N}} = 120 \text{ pm}$
- triple : $d_{\text{N-N}} = 108 \text{ pm}$

1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026	13 B boron 10.811 [10.806, 10.812]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998 [18.998, 18.998]	18 Ne neon 20.180 [20.179, 20.180]
3 Li lithium 6.941 [6.938, 6.944]	4 Be beryllium 9.012 [9.012, 9.012]	5 B boron 10.811 [10.806, 10.812]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998 [18.998, 18.998]	10 Ne neon 20.180 [20.179, 20.180]
11 Na sodium 22.990 [22.989, 22.991]	12 Mg magnesium 24.305 [24.304, 24.306]	13 B boron 10.811 [10.806, 10.812]	14 Si silicon 28.086 [28.085, 28.087]	15 P phosphorus 30.974 [30.972, 30.976]	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948 [39.942, 39.948]
19 K potassium 39.098 [39.096, 39.101]	20 Ca calcium 40.078 [40.078, 40.078]	21 Sc scandium 44.956 [44.955, 44.957]	22 Ti titanium 47.88 [47.877, 47.883]	23 V vanadium 50.942 [50.941, 50.943]	24 Cr chromium 52.00 [51.996, 52.004]	25 Mn manganese 54.938 [54.937, 54.939]	26 Fe iron 55.845 [55.845, 55.845]
27 Co cobalt 58.933 [58.933, 58.933]	28 Ni nickel 58.69 [58.693, 58.697]	29 Cu copper 63.546 [63.546, 63.546]	30 Zn zinc 65.38 [65.376, 65.384]	31 Ga gallium 69.723 [69.723, 69.723]	32 Ge germanium 72.63 [72.630, 72.631]	33 As arsenic 74.922 [74.921, 74.923]	34 Se selenium 78.971 [78.971, 78.972]
35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.798 [83.798, 83.798]	37 Rb rubidium 85.468 [85.468, 85.468]	38 Sr strontium 87.62 [87.62, 87.62]	39 Y yttrium 88.906 [88.906, 88.906]	40 Zr zirconium 91.224 [91.224, 91.224]	41 Nb niobium 92.906 [92.906, 92.906]	42 Mo molybdenum 95.94 [95.94, 95.94]
43 Tc technetium 98.906 [98.906, 98.906]	44 Ru ruthenium 101.07 [101.07, 101.07]	45 Rh rhodium 102.905 [102.905, 102.905]	46 Pd palladium 106.42 [106.42, 106.42]	47 Ag silver 107.868 [107.868, 107.868]	48 Cd cadmium 112.414 [112.414, 112.414]	49 In indium 114.818 [114.818, 114.818]	50 Hg mercury 200.59 [200.59, 200.59]
51 Sb antimony 121.76 [121.76, 121.76]	52 Te tellurium 127.60 [127.60, 127.60]	53 I iodine 126.905 [126.905, 126.905]	54 Xe xenon 131.29 [131.29, 131.29]	55 Ba barium 137.327 [137.327, 137.327]	56 La lanthanum 138.905 [138.905, 138.905]	57 Ce cerium 140.12 [140.12, 140.12]	58 Pr praseodymium 140.91 [140.91, 140.91]
59 Nd neodymium 144.24 [144.24, 144.24]	60 Pm promethium 144.91 [144.91, 144.91]	61 Sm samarium 150.36 [150.36, 150.36]	62 Eu europium 151.96 [151.96, 151.96]	63 Gd gadolinium 157.25 [157.25, 157.25]	64 Tb terbium 158.93 [158.93, 158.93]	65 Dy dysprosium 162.50 [162.50, 162.50]	66 Ho holmium 164.93 [164.93, 164.93]
67 Er erbium 167.26 [167.26, 167.26]	68 Tm thulium 168.93 [168.93, 168.93]	69 Yb ytterbium 173.05 [173.05, 173.05]	70 Lu lutetium 174.97 [174.97, 174.97]	71 Fr francium 223.02 [223.02, 223.02]	72 Ra radium 226.025 [226.025, 226.025]	73 Ac actinoids	74 Rf rutherfordium 261.10 [261.10, 261.10]
75 Db dubnium 262.10 [262.10, 262.10]	76 Sg seaborgium 263.10 [263.10, 263.10]	77 Bh bohrium 264.10 [264.10, 264.10]	78 Hs hassium 265.10 [265.10, 265.10]	79 Mt meitnerium 266.10 [266.10, 266.10]	80 Ds darmstadtium 267.10 [267.10, 267.10]	81 Rg roentgenium 268.10 [268.10, 268.10]	82 Cn copernicium 269.10 [269.10, 269.10]
83 Nh nihonium 270.10 [270.10, 270.10]	84 Fl flerovium 271.10 [271.10, 271.10]	85 Mc moscovium 272.10 [272.10, 272.10]	86 Lv livermorium 273.10 [273.10, 273.10]	87 Ts tennessine 274.10 [274.10, 274.10]	88 Og oganesson 275.10 [275.10, 275.10]	89 Fr francium 223.02 [223.02, 223.02]	90 Ra radium 226.025 [226.025, 226.025]
91 Ac actinium 227.03 [227.03, 227.03]	92 Th thorium 232.04 [232.04, 232.04]	93 Pa protactinium 231.04 [231.04, 231.04]	94 U uranium 238.03 [238.03, 238.03]	95 Np neptunium 237.05 [237.05, 237.05]	96 Pu plutonium 244.06 [244.06, 244.06]	97 Am americium 243.06 [243.06, 243.06]	98 Cm curium 247.07 [247.07, 247.07]
99 Bk berkelium 247.07 [247.07, 247.07]	100 Cf californium 251.08 [251.08, 251.08]	101 Es einsteinium 252.08 [252.08, 252.08]	102 Fm fermium 257.10 [257.10, 257.10]	103 Md mendelevium 258.10 [258.10, 258.10]	104 No nobelium 259.10 [259.10, 259.10]	105 Lr lawrencium 260.10 [260.10, 260.10]	106 Uu unbinilium 289.10 [289.10, 289.10]
107 Uub unbinilium 288.10 [288.10, 288.10]	108 Uuq unquincium 289.10 [289.10, 289.10]	109 Uub unbinilium 288.10 [288.10, 288.10]	110 Uuq unquincium 289.10 [289.10, 289.10]	111 Uub unbinilium 288.10 [288.10, 288.10]	112 Uuq unquincium 289.10 [289.10, 289.10]	113 Uub unbinilium 288.10 [288.10, 288.10]	114 Uuq unquincium 289.10 [289.10, 289.10]
115 Uub unbinilium 288.10 [288.10, 288.10]	116 Uuq unquincium 289.10 [289.10, 289.10]	117 Uub unbinilium 288.10 [288.10, 288.10]	118 Uuq unquincium 289.10 [289.10, 289.10]	119 Uub unbinilium 288.10 [288.10, 288.10]	120 Uuq unquincium 289.10 [289.10, 289.10]	121 Uub unbinilium 288.10 [288.10, 288.10]	122 Uuq unquincium 289.10 [289.10, 289.10]

Molecular solids under Pressure :

1. Squeezing the « van der Waals space »
2. Increasing coordination numbers
3. Shortening bonds
4. Electrons moving off their atoms



Polymerization

For notes and updates to this table, see www.iupac.org. This version is dated 28 November 2016. Copyright © 2016 IUPAC, the International Union of Pure and Applied Chemistry.

What about Hydrogen ?

IUPAC Periodic Table of the Elements

Key: atomic number, Symbol, name

NITROGEN

$P = 1 \text{ atm}$

$\alpha\text{-N}_2$ (molecular)
CN = 1 ($d_{\text{N-N}} = 106 \text{ pm}$)

$P \uparrow$

$P = 115 \text{ GPa}$

Cubic gauche N (monatomic)
CN = 3 ($d_{\text{N-N}} = 146 \text{ pm}$)

- single : $d_{\text{N-N}} = 142 \text{ pm}$
- double: $d_{\text{N-N}} = 120 \text{ pm}$
- triple : $d_{\text{N-N}} = 108 \text{ pm}$

1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026	13 B boron 10.811 [10.806, 10.812]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998	18 Ne neon 20.180
3 Li lithium 6.941 [6.938, 6.944]	4 Be beryllium 9.0122	5 B boron 10.811 [10.806, 10.812]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990 [22.989, 22.991]	12 Mg magnesium 24.305 [24.304, 24.306]	13 Al aluminum 26.982 [26.981, 26.983]	14 Si silicon 28.086 [28.085, 28.087]	15 P phosphorus 30.974 [30.972, 30.976]	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098 [39.096, 39.101]	20 Ca calcium 40.078 [40.078, 40.078]	21 Sc scandium 44.956 [44.955, 44.957]	22 Ti titanium 47.88 [47.877, 47.883]	23 V vanadium 50.942 [50.941, 50.943]	24 Cr chromium 52.004 [51.996, 52.002]	25 Mn manganese 54.938 [54.937, 54.939]	26 Fe iron 55.845 [55.845, 55.845]
27 Co cobalt 58.933 [58.933, 58.933]	28 Ni nickel 58.693 [58.693, 58.693]	29 Cu copper 63.546 [63.546, 63.546]	30 Zn zinc 65.38 [65.38, 65.38]	31 Ga gallium 69.723 [69.723, 69.723]	32 Ge germanium 72.63 [72.63, 72.63]	33 As arsenic 74.922 [74.922, 74.922]	34 Se selenium 78.9718 [78.9718, 78.9718]
35 Br bromine 79.904 [79.904, 79.904]	36 Kr krypton 83.798 [83.798, 83.798]	37 Rb rubidium 85.468 [85.468, 85.468]	38 Sr strontium 87.62 [87.62, 87.62]	39 Y yttrium 88.906 [88.906, 88.906]	40 Zr zirconium 91.224 [91.224, 91.224]	41 Nb niobium 92.906 [92.906, 92.906]	42 Mo molybdenum 95.94 [95.94, 95.94]
43 Tc technetium 98.906 [98.906, 98.906]	44 Ru ruthenium 101.07 [101.07, 101.07]	45 Rh rhodium 102.905 [102.905, 102.905]	46 Pd palladium 106.42 [106.42, 106.42]	47 Ag silver 107.868 [107.868, 107.868]	48 Cd cadmium 112.411 [112.411, 112.411]	49 In indium 114.818 [114.818, 114.818]	50 Sn tin 118.710 [118.710, 118.710]
51 Sb antimony 121.76 [121.76, 121.76]	52 Te tellurium 127.603 [127.603, 127.603]	53 I iodine 126.905 [126.905, 126.905]	54 Xe xenon 131.29 [131.29, 131.29]	55 Ba barium 137.327 [137.327, 137.327]	56 La lanthanum 138.905 [138.905, 138.905]	57 Ce cerium 140.12 [140.12, 140.12]	58 Pr praseodymium 140.91 [140.91, 140.91]
59 Nd neodymium 144.24 [144.24, 144.24]	60 Pm promethium 144.913 [144.913, 144.913]	61 Sm samarium 150.36 [150.36, 150.36]	62 Eu europium 151.96 [151.96, 151.96]	63 Gd gadolinium 157.25 [157.25, 157.25]	64 Tb terbium 158.93 [158.93, 158.93]	65 Dy dysprosium 162.50 [162.50, 162.50]	66 Ho holmium 164.93 [164.93, 164.93]
67 Er erbium 167.26 [167.26, 167.26]	68 Tm thulium 168.93 [168.93, 168.93]	69 Yb ytterbium 173.05 [173.05, 173.05]	70 Lu lutetium 174.97 [174.97, 174.97]	71 Hf hafnium 178.49 [178.49, 178.49]	72 Ta tantalum 180.948 [180.948, 180.948]	73 W tungsten 183.84 [183.84, 183.84]	74 Re rhenium 186.207 [186.207, 186.207]
75 Os osmium 190.23 [190.23, 190.23]	76 Ir iridium 192.22 [192.22, 192.22]	77 Pt platinum 195.084 [195.084, 195.084]	78 Au gold 196.967 [196.967, 196.967]	79 Hg mercury 200.59 [200.59, 200.59]	80 Tl thallium 204.38 [204.38, 204.38]	81 Pb lead 207.2 [207.2, 207.2]	82 Bi bismuth 208.98 [208.98, 208.98]
83 Po polonium 209 [209, 209]	84 At astatine 210 [210, 210]	85 Rn radon 222 [222, 222]	86 Fr francium 223 [223, 223]	87 Ra radium 226 [226, 226]	88 Ac actinium 227.03 [227.03, 227.03]	89 Th thorium 232.04 [232.04, 232.04]	90 Pa protactinium 231.04 [231.04, 231.04]
91 U uranium 238.03 [238.03, 238.03]	92 Np neptunium 237.05 [237.05, 237.05]	93 Pu plutonium 244 [244, 244]	94 Am americium 243 [243, 243]	95 Cm curium 247 [247, 247]	96 Bk berkelium 247 [247, 247]	97 Cf californium 251 [251, 251]	98 Es einsteinium 252 [252, 252]
99 Fm fermium 257 [257, 257]	100 Md mendelevium 258 [258, 258]	101 No nobelium 259 [259, 259]	102 Lr lawrencium 260 [260, 260]	103 Rf rutherfordium 261 [261, 261]	104 Db dubnium 262 [262, 262]	105 Sg seaborgium 263 [263, 263]	106 Bh bohrium 264 [264, 264]
107 Hs hassium 265 [265, 265]	108 Mt meitnerium 266 [266, 266]	109 Ds darmstadtium 268 [268, 268]	110 Rg roentgenium 269 [269, 269]	111 Cn copernicium 277 [277, 277]	112 Nh nihonium 278 [278, 278]	113 Fl flerovium 285 [285, 285]	114 Mc moscovium 285 [285, 285]
115 Lv livermorium 286 [286, 286]	116 Ts tennessine 287 [287, 287]	117 Og oganesson 289 [289, 289]	118 Og oganesson 289 [289, 289]	119 Uue unbinilium 289 [289, 289]	120 Uub unbinilium 289 [289, 289]	121 Uut ununilium 289 [289, 289]	122 Uuq ununilium 289 [289, 289]
123 Uup ununilium 289 [289, 289]	124 Uuq ununilium 289 [289, 289]	125 Uup ununilium 289 [289, 289]	126 Uuq ununilium 289 [289, 289]	127 Uup ununilium 289 [289, 289]	128 Uuq ununilium 289 [289, 289]	129 Uup ununilium 289 [289, 289]	130 Uuq ununilium 289 [289, 289]

Molecular solids under Pressure :

1. Squeezing the « van der Waals space »
2. Increasing coordination numbers
3. Shortening bonds
4. Electrons moving off their atoms

Polymerization

What about Hydrogen ?

IUPAC Periodic Table of the Elements

Key:
 atomic number
Symbol
 name
 conventional atomic weight
 standard atomic weight

1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026											13 B boron 10.81 [10.806, 10.821]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998	18 Ne neon 20.180
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.089]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]	3	4	5	6	7	8	9	10	11	12	13 Ga gallium 69.723	14 Ge germanium 72.630(8)	15 As arsenic 74.922	16 Se selenium 78.971(8)	17 Br bromine 79.904 [79.901, 79.907]	18 Kr krypton 83.796(2)
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.796(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Same behavior expected
(P-induced polymerization)

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

What about Hydrogen ?

IUPAC Periodic Table of the Elements

Key:
 atomic number
Symbol
 name
 conventional atomic weight
 standard atomic weight

1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026											13 B boron 10.81 [10.806, 10.821]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998	18 Ne neon 20.180
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.806, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]	3	4	5	6	7	8	9	10	11	12	13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.089]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.798(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Same behavior expected
(P-induced polymerization)

- Structural modifications induced by P not so easy to characterize experimentally (weak X-ray scattering)

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

What about Hydrogen ?

IUPAC Periodic Table of the Elements

Key:
 atomic number
Symbol
 name
 conventional atomic weight
 standard atomic weight

1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026											13 B boron 10.81 [10.806, 10.821]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998	18 Ne neon 20.180
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.806, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]	3	4	5	6	7	8	9	10	11	12	13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.088]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.798(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Same behavior expected
(P-induced polymerization)

- Structural modifications induced by P not so easy to characterize experimentally (weak X-ray scattering)
- P required to induce H₂ dissociation much higher than expected initially

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

What about Hydrogen ?

Double motivation

IUPAC Periodic Table of the Elements

Key:
 atomic number
Symbol
 name
 conventional atomic weight
 standard atomic weight

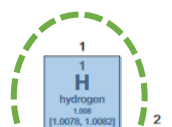
1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026											13 B boron 10.81 [10.806, 10.821]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998	18 Ne neon 20.180
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.806, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]	3	4	5	6	7	8	9	10	11	12	13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.088]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.798(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

- H : 1st element
- H-H bond : prototypical 2e-2c covalent bond

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

What about Hydrogen ?

IUPAC Periodic Table of the Elements



1												18					
1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026											13	14	15	16	17	10
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.806, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.000]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]											13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.088]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.448, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.796(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium 101.07(2)	44 Ru ruthenium 102.91	45 Rh rhodium 106.42	46 Pd palladium 107.87	47 Ag silver 112.41	48 Cd cadmium 114.82	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Key:
atomic number
Symbol
name
conventional atomic weight
standard atomic weight

Double motivation

- H : 1st element
- H-H bond : prototypical 2e-2c covalent bond

A key to understand the behavior of bonds under pressure

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

What about Hydrogen ?

IUPAC Periodic Table of the Elements

Key:

atomic number	Symbol	name
conventional atomic weight		
standard atomic weight		

Double motivation

- H : 1st element
- H-H bond : prototypical 2e-2c covalent bond

A key to understand the behavior of bonds under pressure

- « Polymerized H » should be a metal with appealing properties
 - High T superconductor
 - Metallic superfluid

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
88 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

What about Hydrogen ?

IUPAC Periodic Table of the Elements

Key:
 atomic number
Symbol
 name
 conventional atomic weight
 standard atomic weight

1 H hydrogen 1.008 [1.0078, 1.0082]	2 He helium 4.0026											13 B boron 10.81 [10.806, 10.821]	14 C carbon 12.011 [12.009, 12.012]	15 N nitrogen 14.007 [14.006, 14.008]	16 O oxygen 15.999 [15.998, 15.999]	17 F fluorine 18.998	18 Ne neon 20.180
3 Li lithium 6.94 [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron 10.81 [10.806, 10.821]	6 C carbon 12.011 [12.009, 12.012]	7 N nitrogen 14.007 [14.006, 14.008]	8 O oxygen 15.999 [15.998, 15.999]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium 24.305 [24.304, 24.307]	3	4	5	6	7	8	9	10	11	12	13 Al aluminium 26.982	14 Si silicon 28.086 [28.084, 28.088]	15 P phosphorus 30.974	16 S sulfur 32.06 [32.059, 32.076]	17 Cl chlorine 35.45 [35.446, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine 79.904 [79.901, 79.907]	36 Kr krypton 83.796(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium 204.38 [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Double motivation

- H : 1st element
- H-H bond : prototypical 2e-2c covalent bond

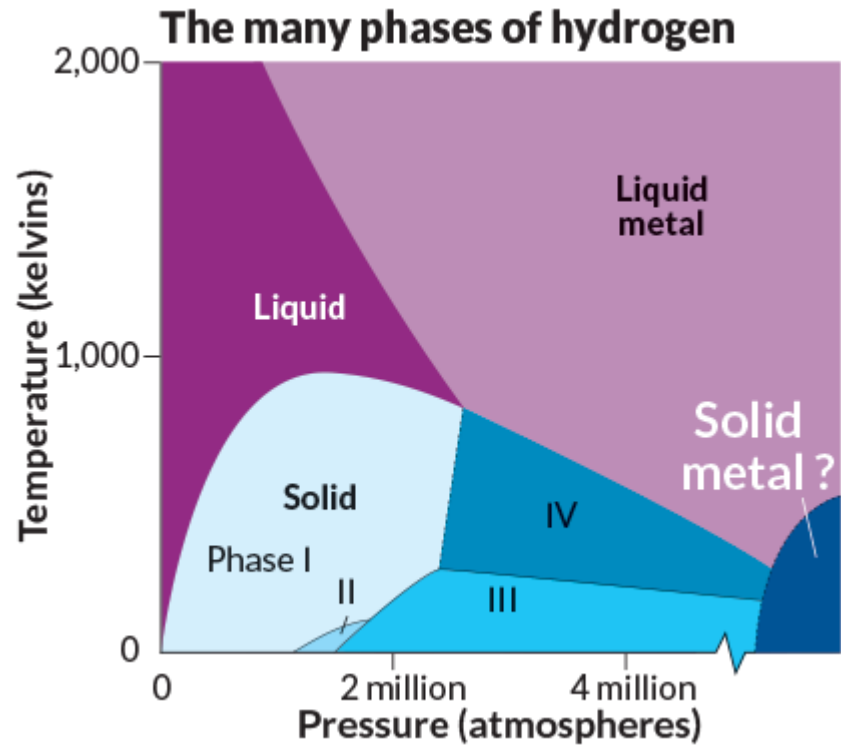
A key to understand the behavior of bonds under pressure

- « Polymerized H » should be a metal with appealing properties
 - High T superconductor
 - Metallic superfluid

Holly Grail of physics

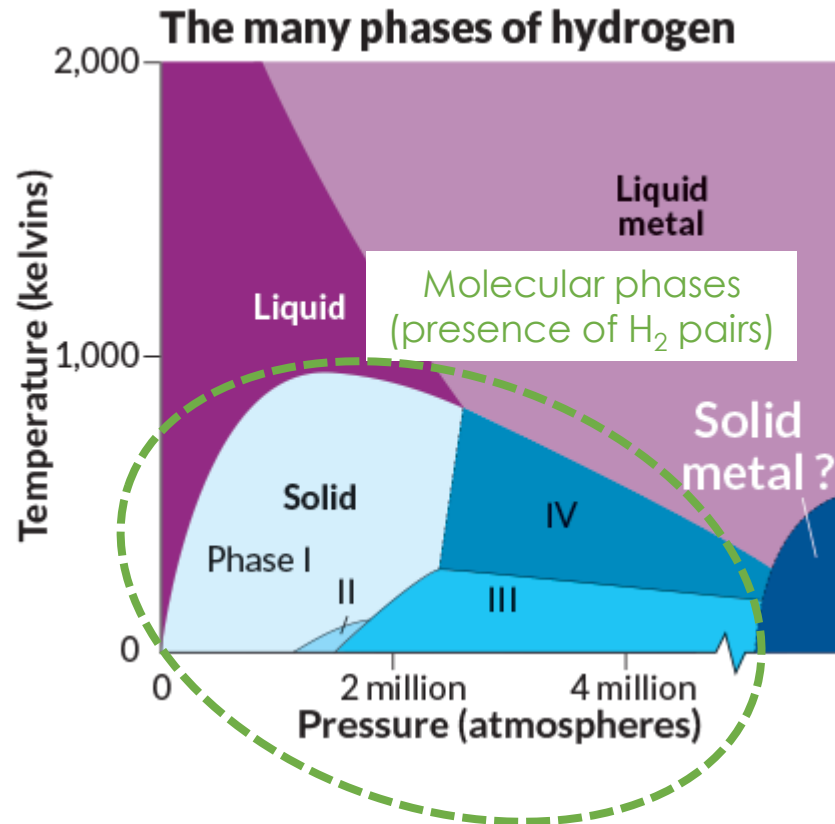
57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
88 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

Dense solid hydrogen - Summary



Source : I.F. Silvera/Harvard Univ. - Adapted by E. Cononver and J. Hirshfeld
(<https://www.sciencenews.org/article/pressure-make-metallic-hydrogen>)

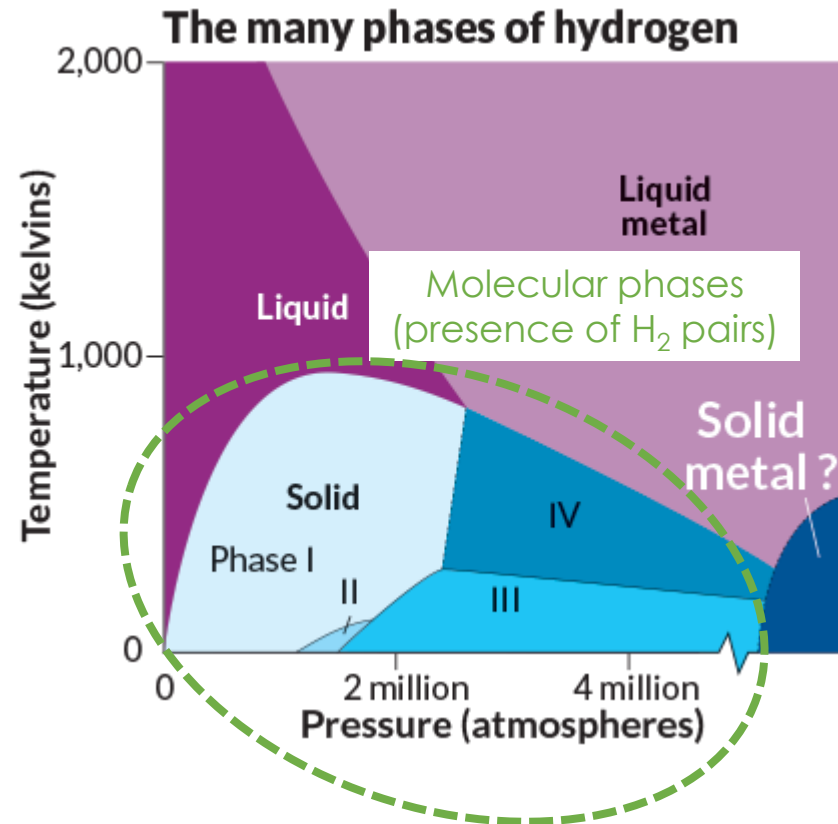
Dense solid hydrogen - Summary



- 4 **molecular phases** known at low T, as P ↗
 - I : H₂ freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib

Source : I.F. Silvera/Harvard Univ. - Adapted by E. Cononver and J. Hirshfeld
(<https://www.sciencenews.org/article/pressure-make-metallic-hydrogen>)

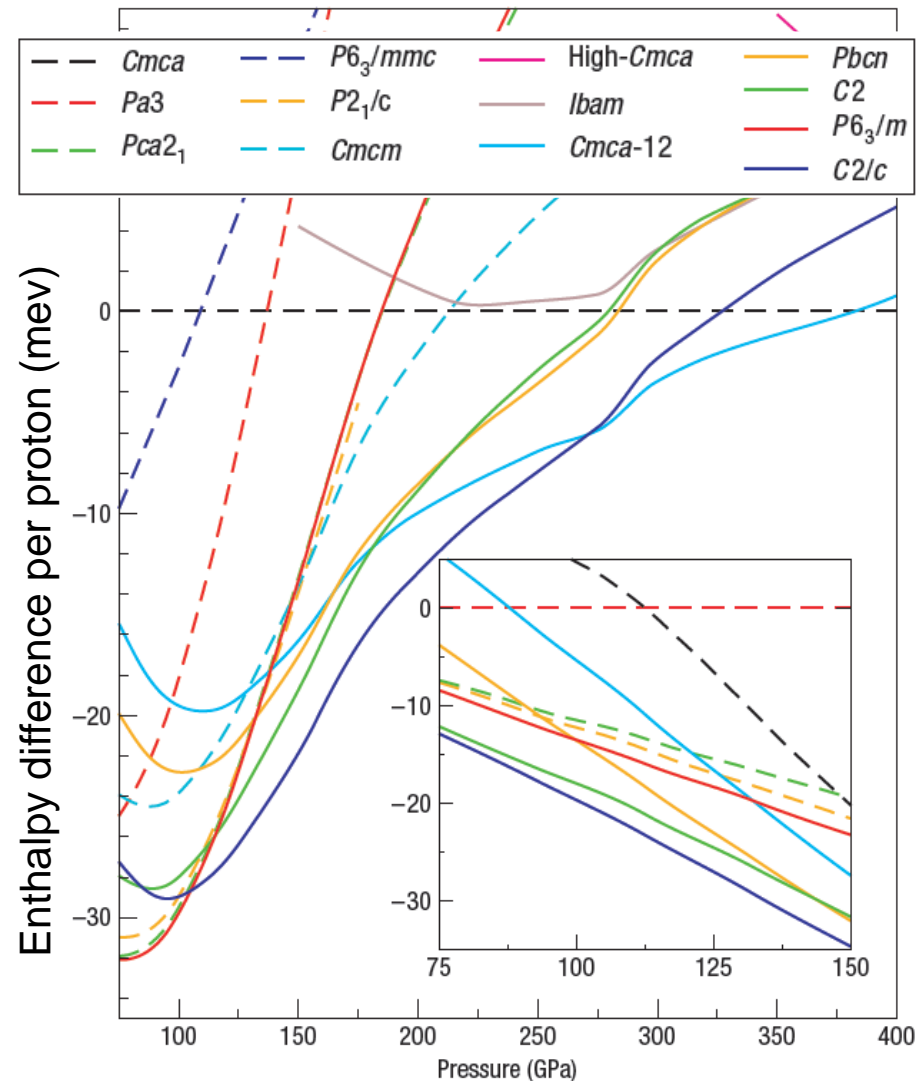
Dense solid hydrogen - Summary



- 4 **molecular phases** known at low T, as P ↗
 - I : H₂ freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib
- Use of numerical simulation coupled to **evolutionary algorithms** to propose **structural models**

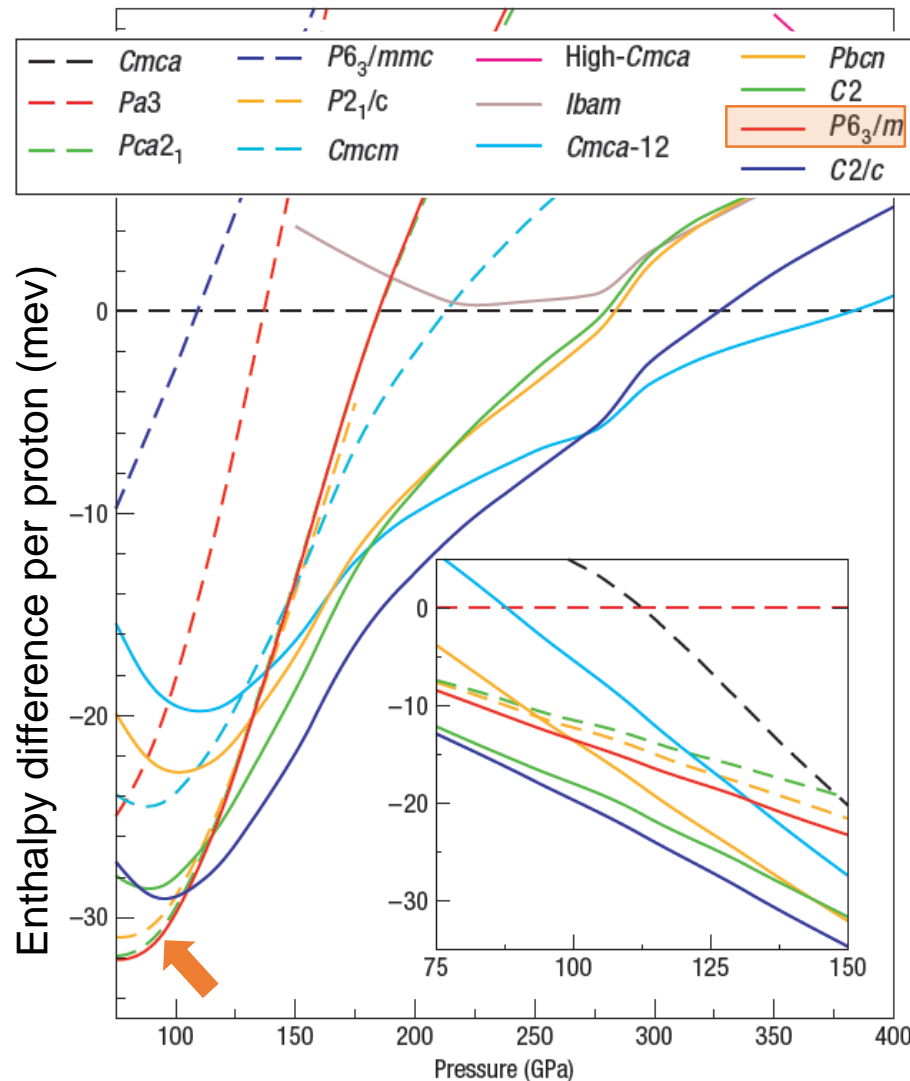
Source : I.F. Silvera/Harvard Univ. - Adapted by E. Cononver and J. Hirshfeld (<https://www.sciencenews.org/article/pressure-make-metallic-hydrogen>)

Dense solid hydrogen - Summary



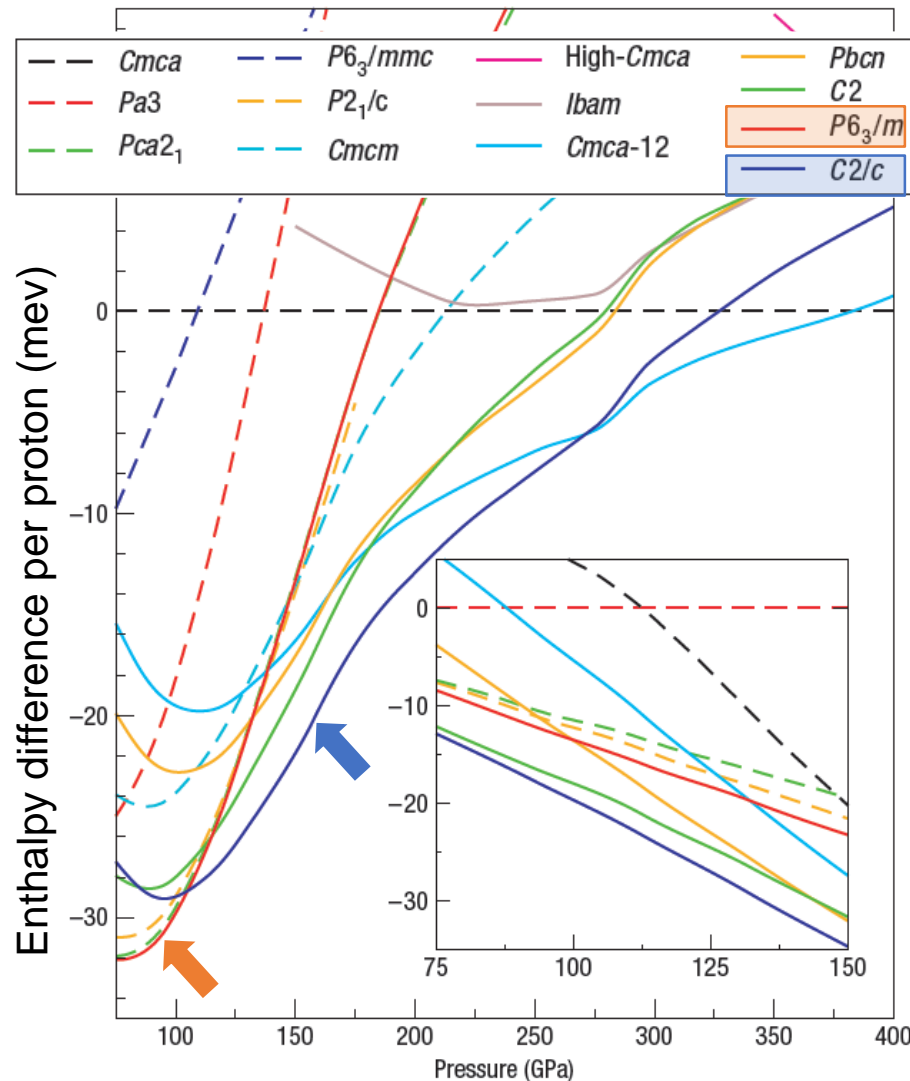
- 4 **molecular phases** known at low T, as $P \nearrow$
 - I : H₂ freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib
- Use of numerical simulation coupled to **evolutionary algorithms** to propose **structural models**
 - Many structures **very close in enthalpy**
 - **Interactions** responsible for the coesion are **essentially the same**
 - Essentially **the same response to $P \nearrow$**

Dense solid hydrogen - Summary



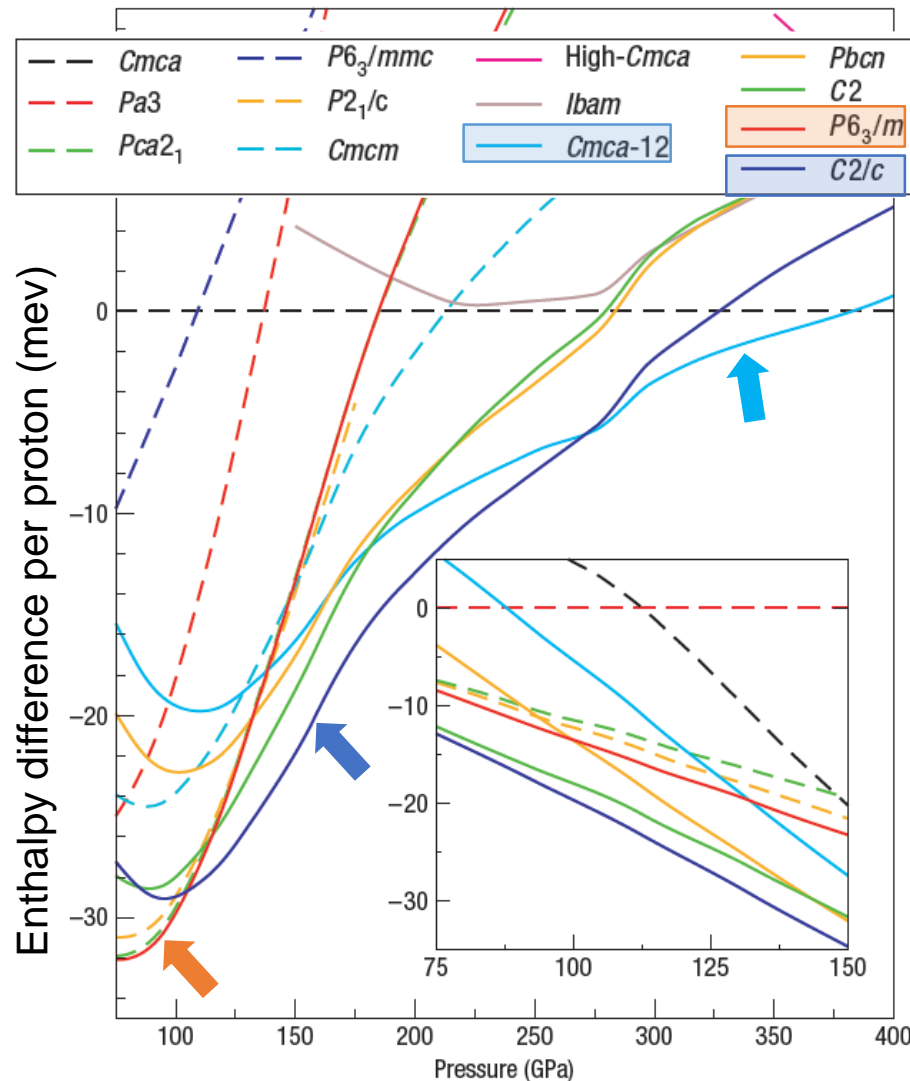
- 4 **molecular phases** known at low T, as $P \nearrow$
 - I : H_2 freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib
- Use of numerical simulation coupled to **evolutionary algorithms** to propose **structural models**
 - Many structures **very close in enthalpy**
 - **Interactions** responsible for the coesion are **essentially the same**
 - Essentially **the same response to $P \nearrow$**

Dense solid hydrogen - Summary



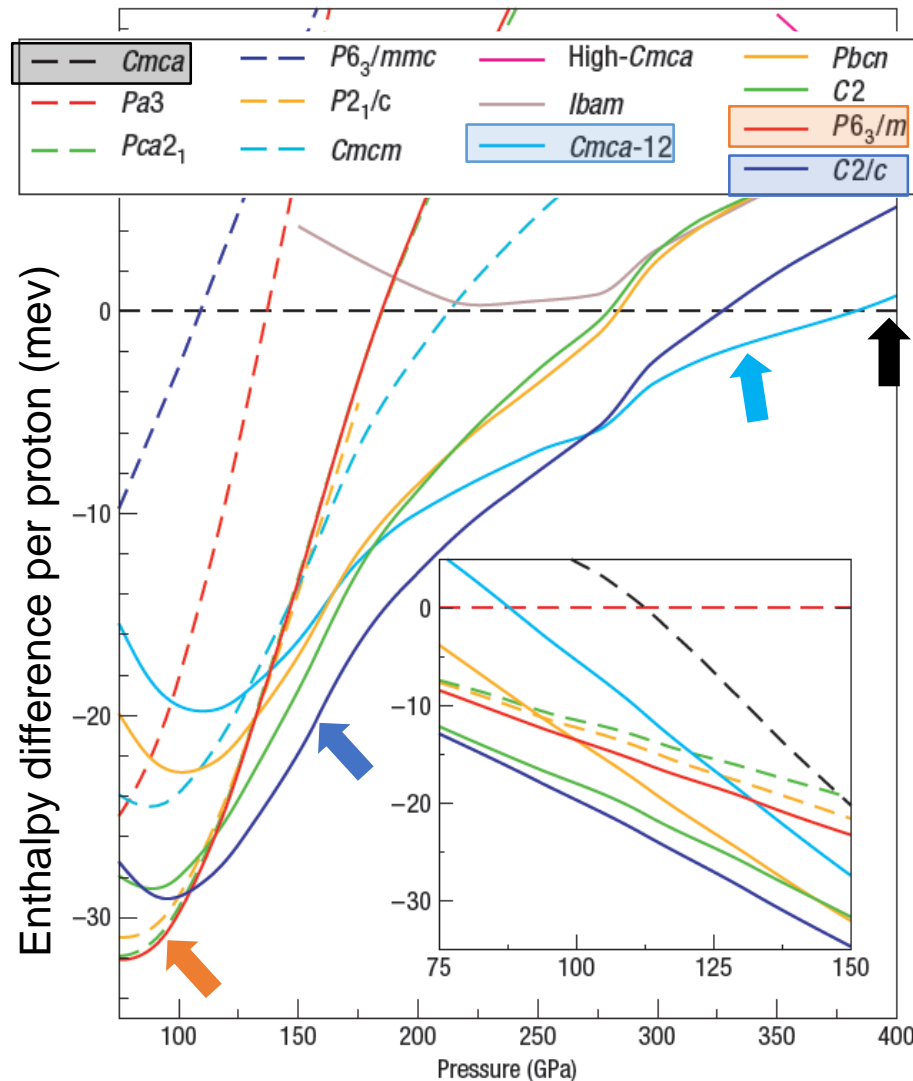
- 4 **molecular phases** known at low T, as $P \nearrow$
 - I : H_2 freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib
- Use of numerical simulation coupled to **evolutionary algorithms** to propose **structural models**
 - Many structures **very close in enthalpy**
 - **Interactions** responsible for the coesion are **essentially the same**
 - Essentially **the same response to $P \nearrow$**

Dense solid hydrogen - Summary



- 4 **molecular phases** known at low T, as $P \nearrow$
 - I : H_2 freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib
- Use of numerical simulation coupled to **evolutionary algorithms** to propose **structural models**
 - Many structures **very close in enthalpy**
 - **Interactions** responsible for the coesion are **essentially the same**
 - Essentially **the same response to $P \nearrow$**

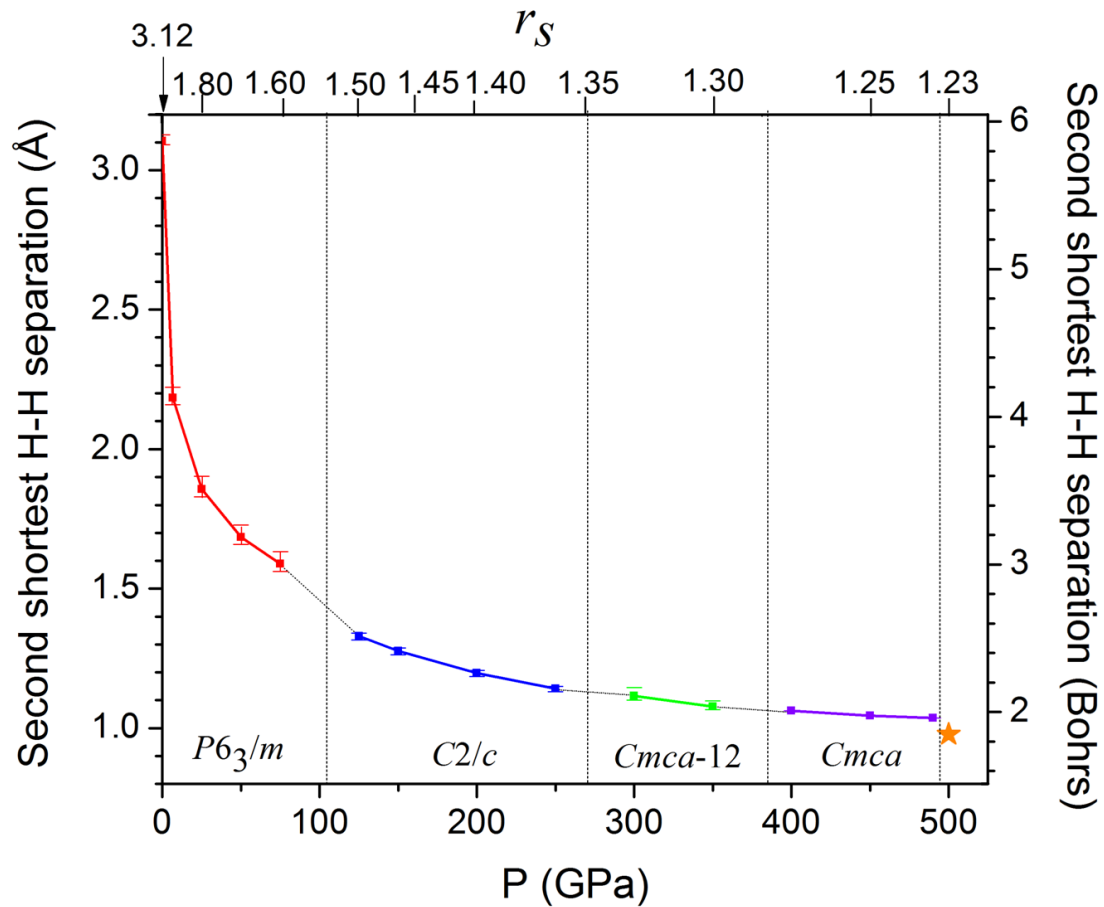
Dense solid hydrogen - Summary



- 4 **molecular phases** known at low T, as $P \nearrow$
 - I : H_2 freely rotating
 - II : orientational ordering
 - III : softening of the intramolecular vib
- Use of numerical simulation coupled to **evolutionary algorithms** to propose **structural models**
 - Many structures **very close in enthalpy**
 - **Interactions** responsible for the coesion are **essentially the same**
 - Essentially **the same response to $P \nearrow$**

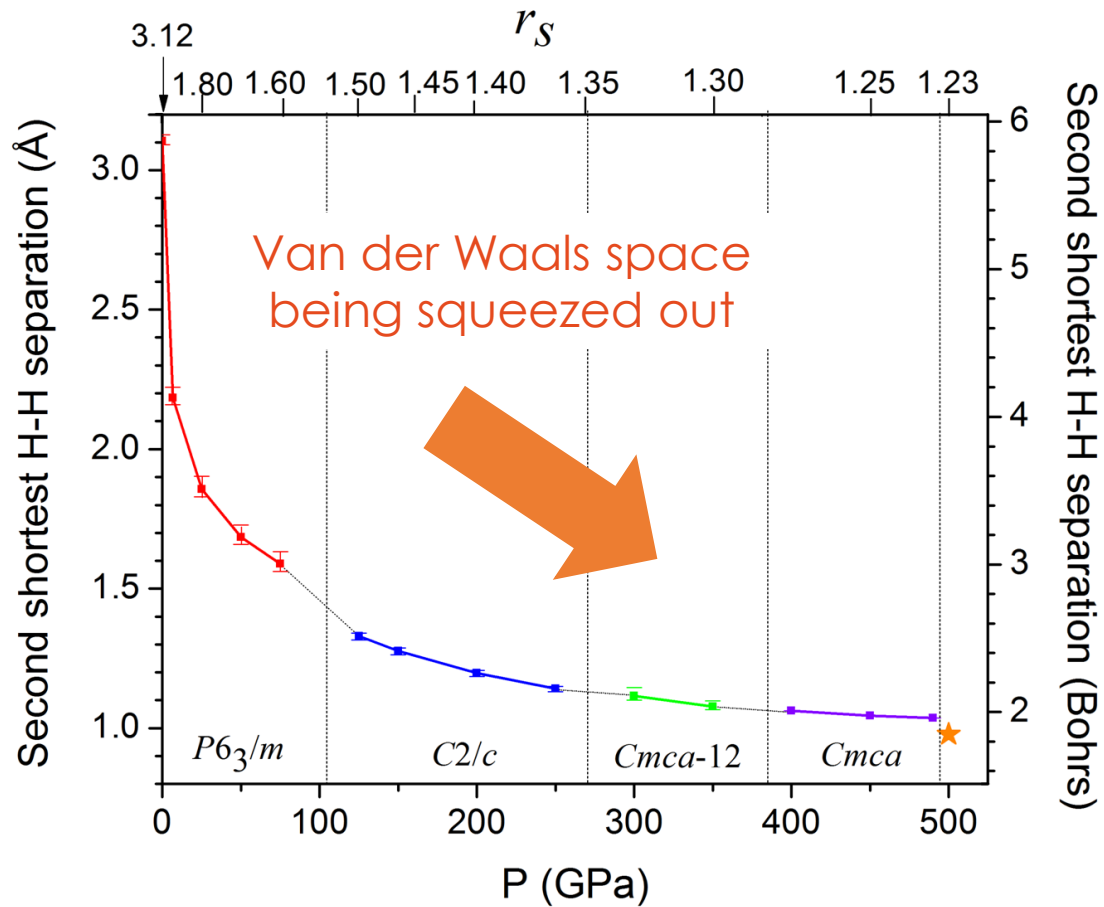
Inter- and intramolecular H-H separations

Intermolecular



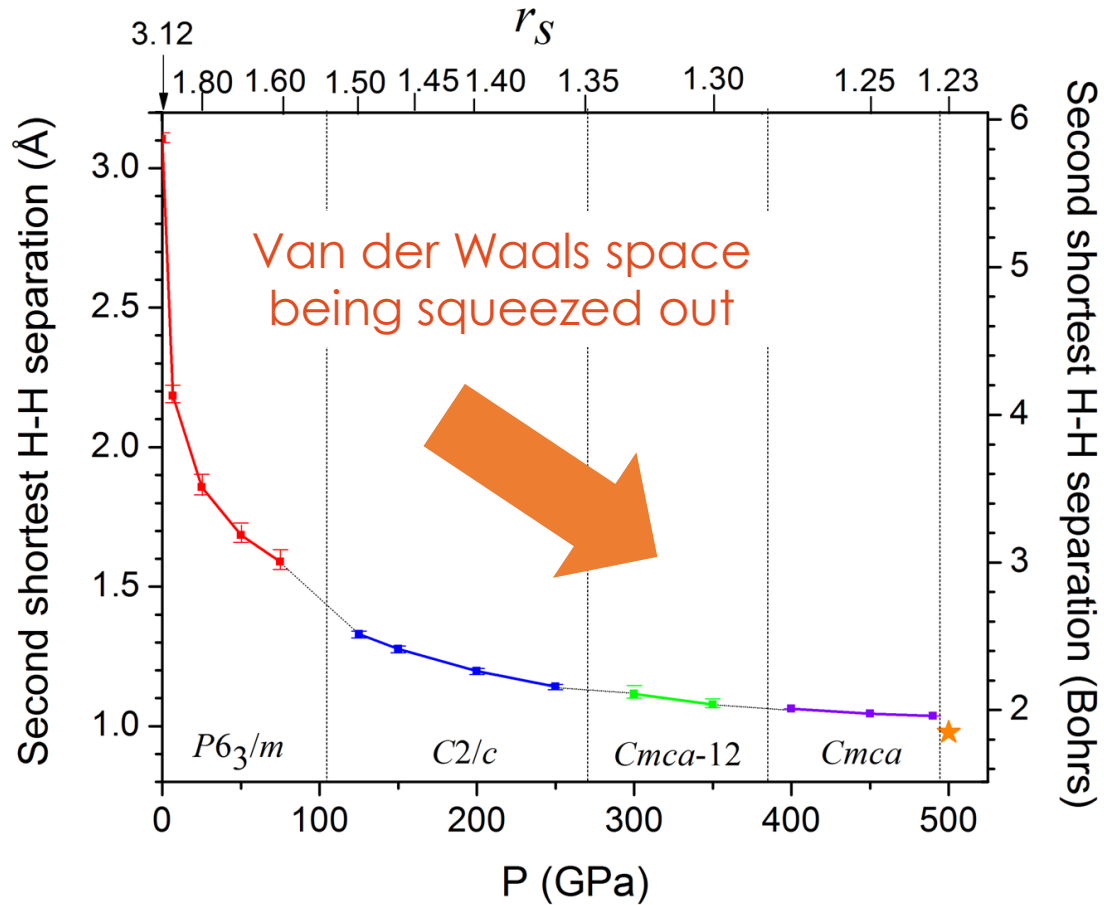
Inter- and intramolecular H-H separations

Intermolecular

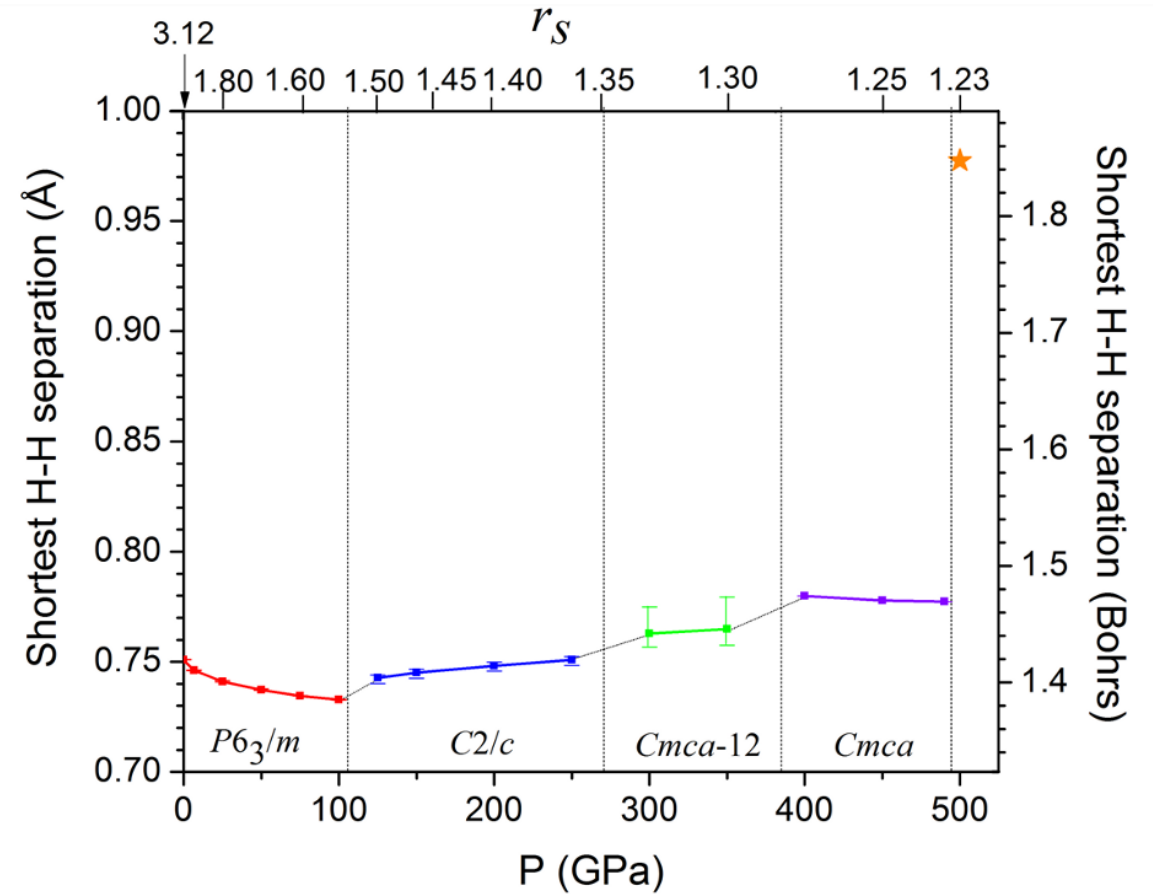


Inter- and intramolecular H-H separations

Intermolecular

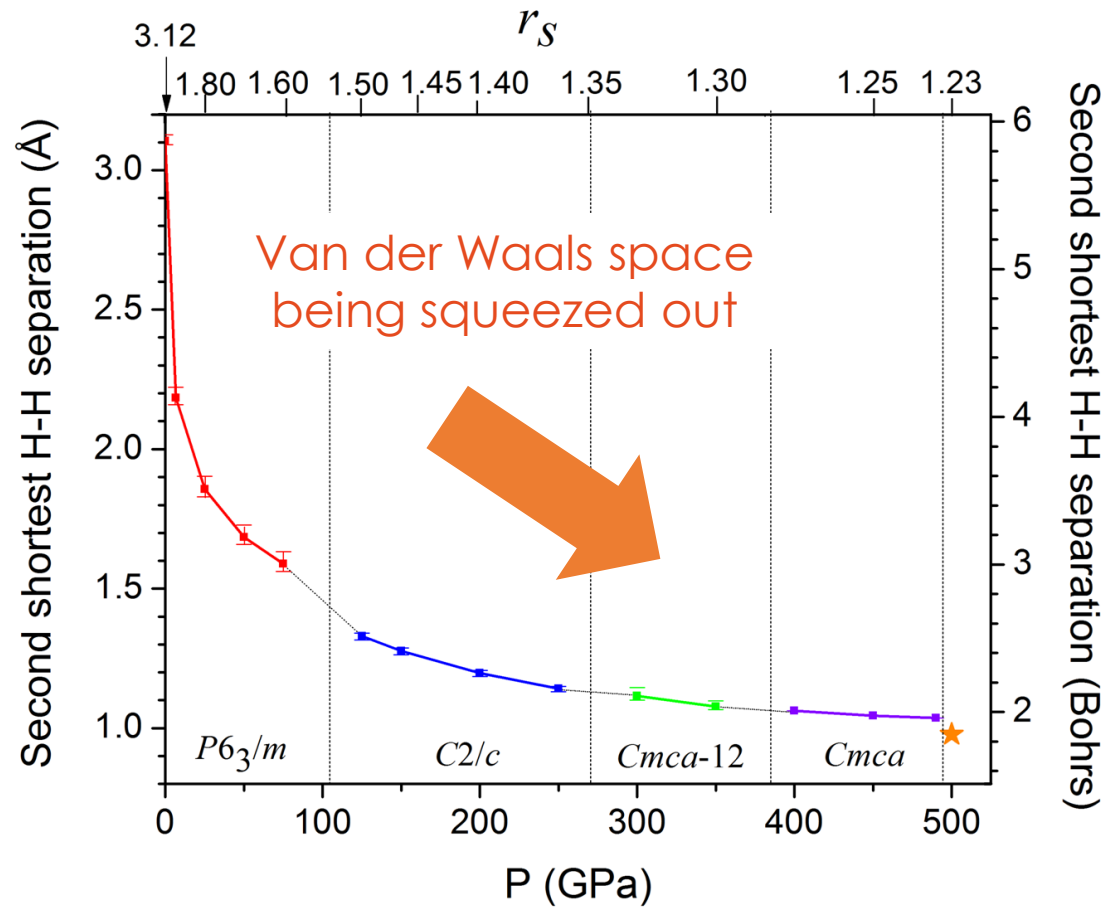


Intramolecular

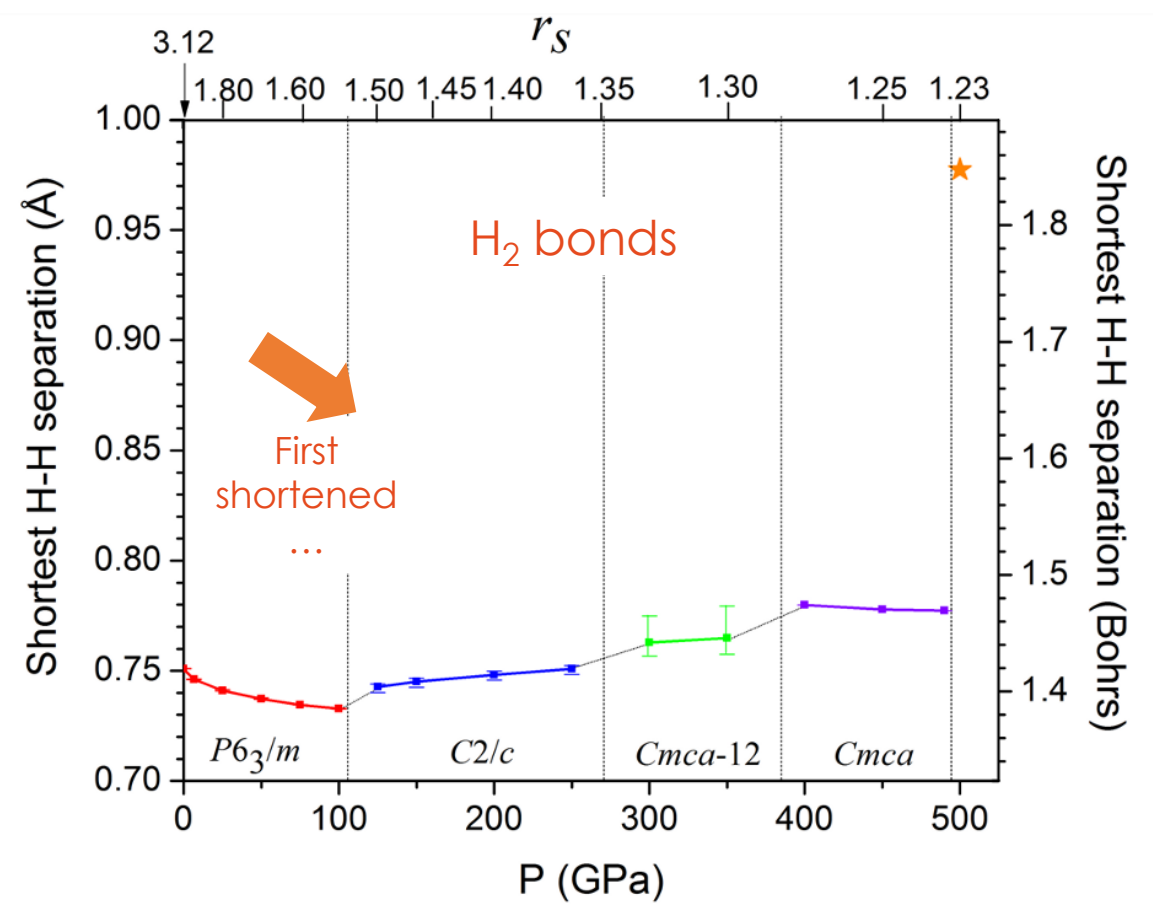


Inter- and intramolecular H-H separations

Intermolecular

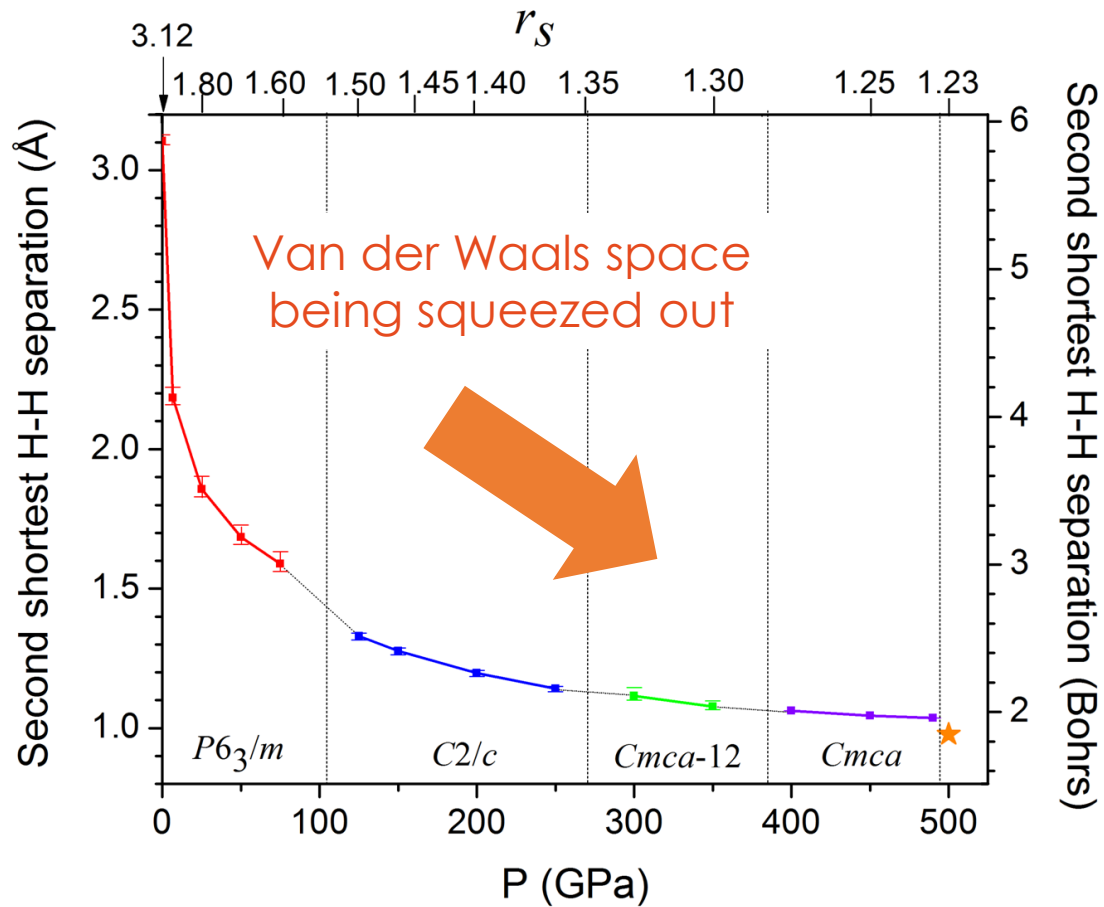


Intramolecular

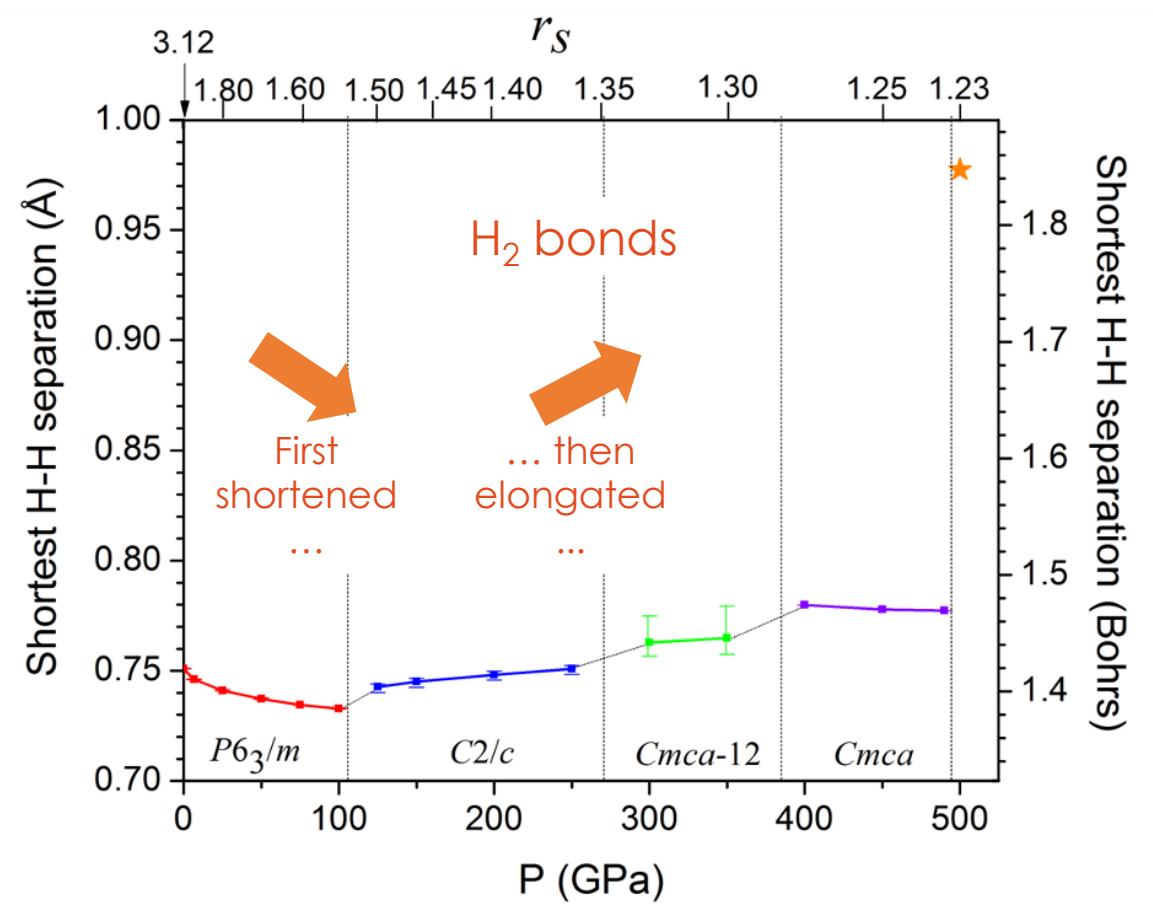


Inter- and intramolecular H-H separations

Intermolecular

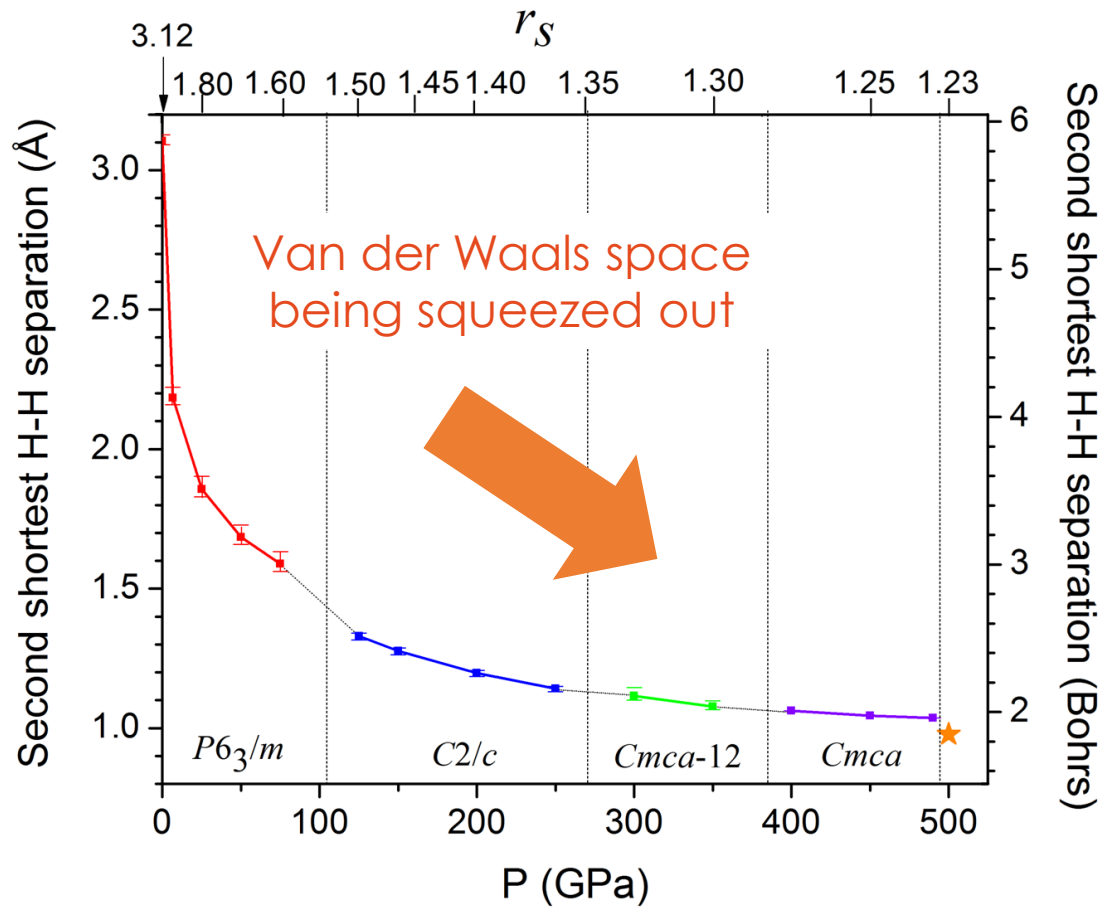


Intramolecular

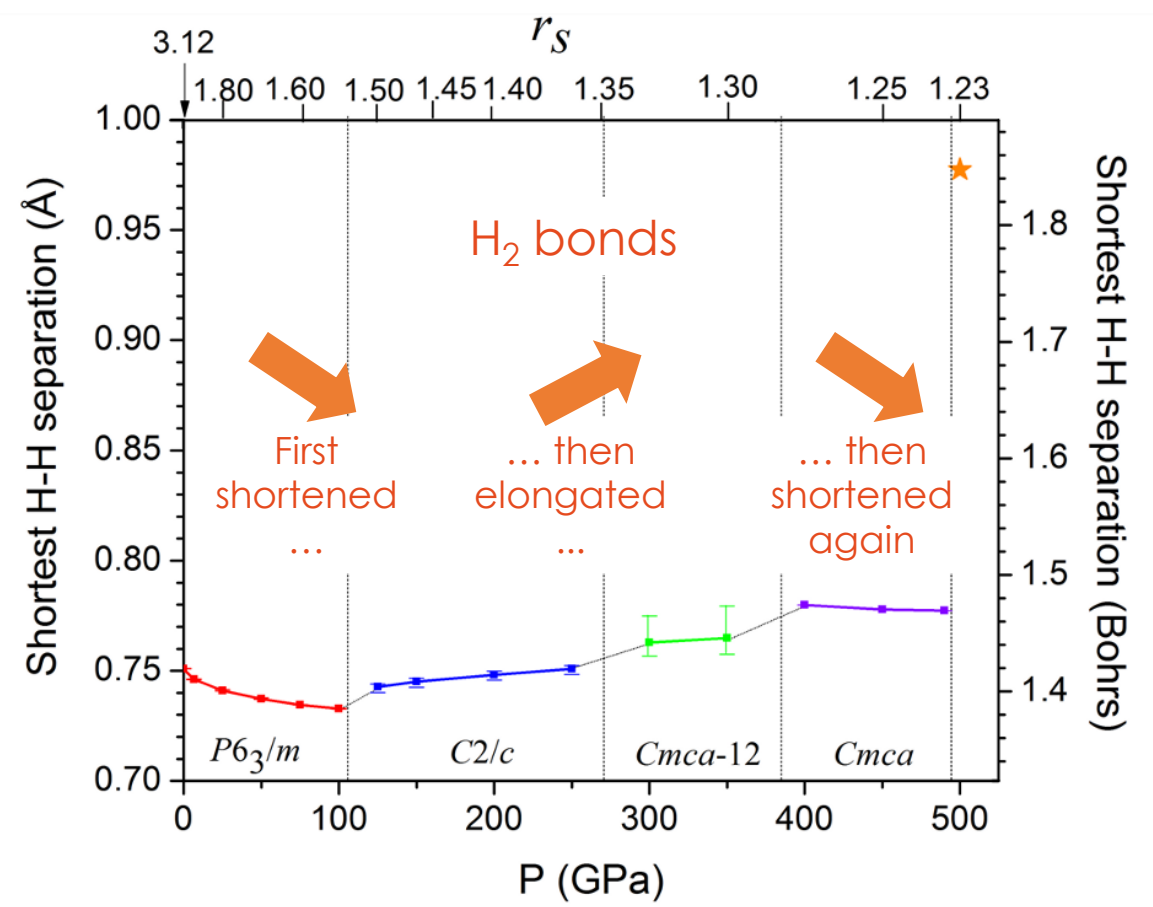


Inter- and intramolecular H-H separations

Intermolecular

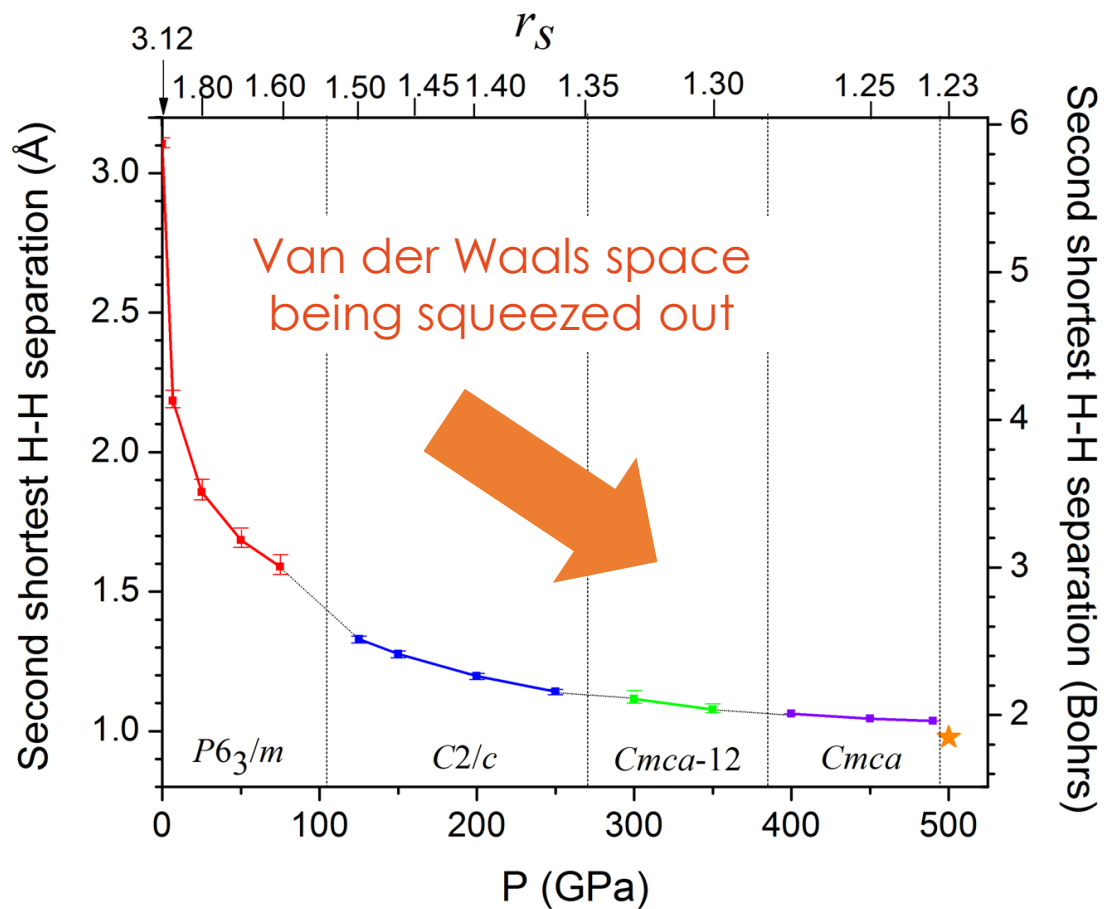


Intramolecular

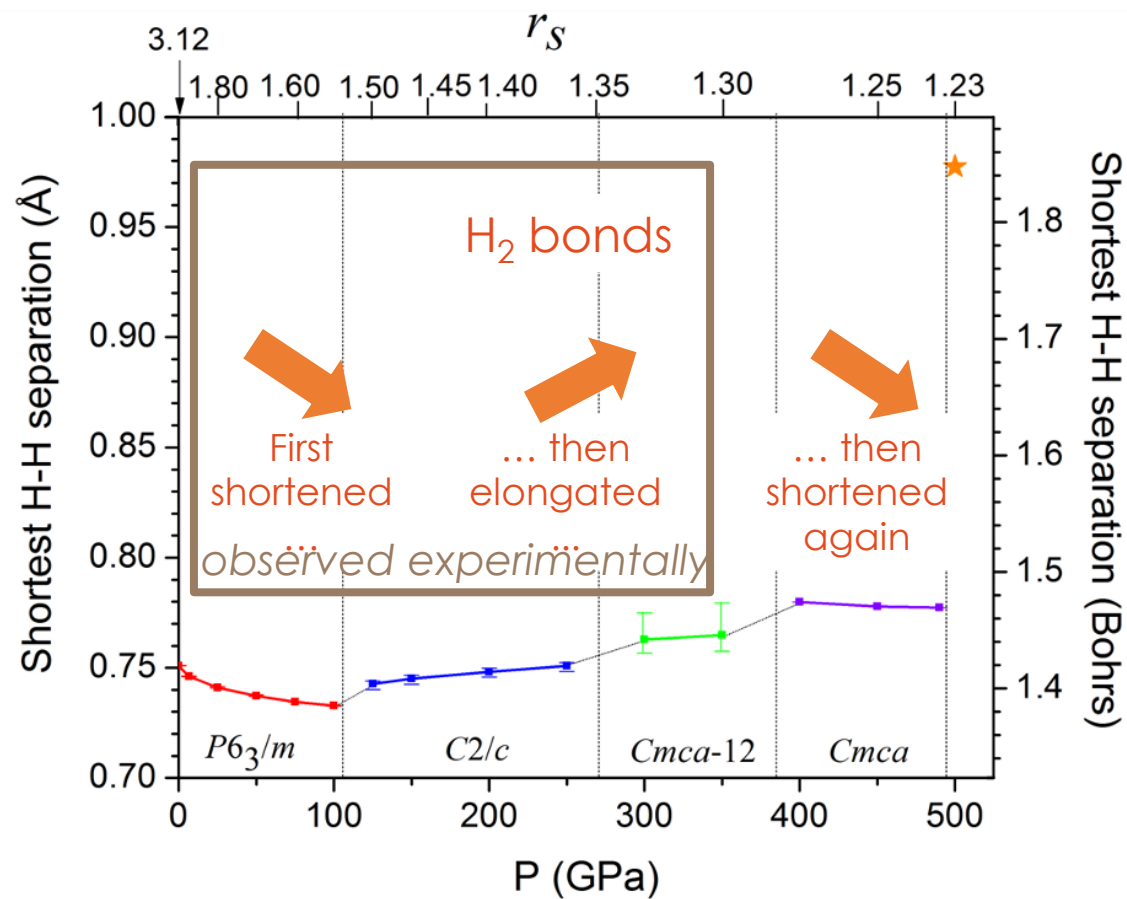


Inter- and intramolecular H-H separations

Intermolecular



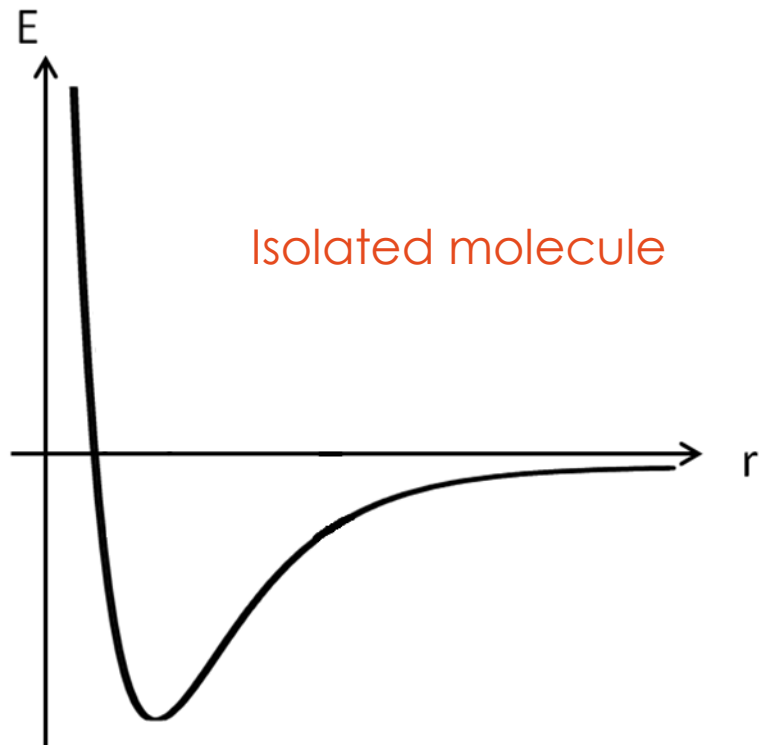
Intramolecular



Bond shortening - The physical wall

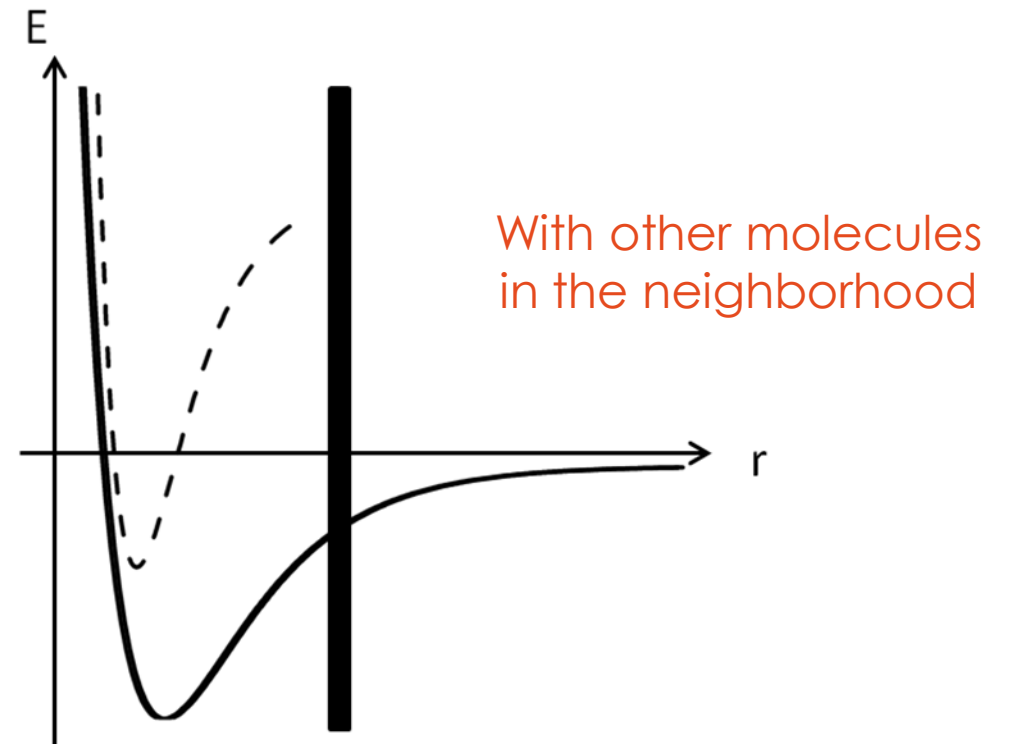
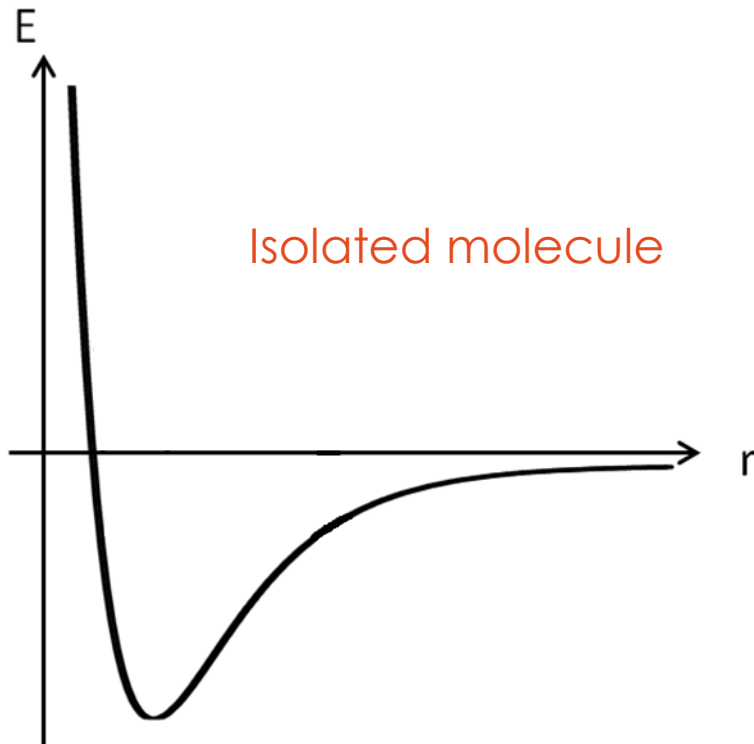
Diatomic molecule

Potential Energy Curve

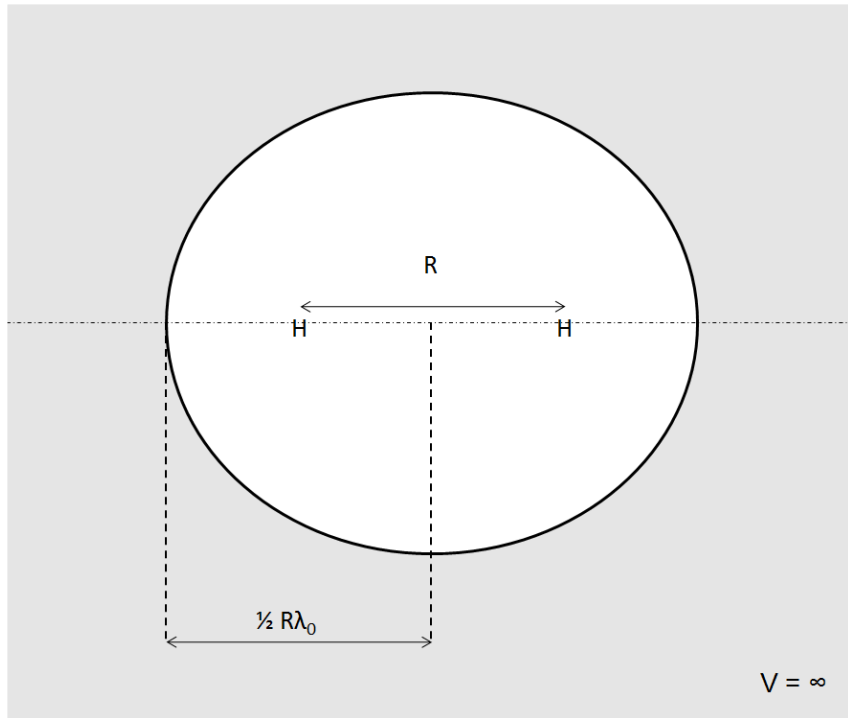


Bond shortening - The physical wall

Diatomic molecule
Potential Energy Curve

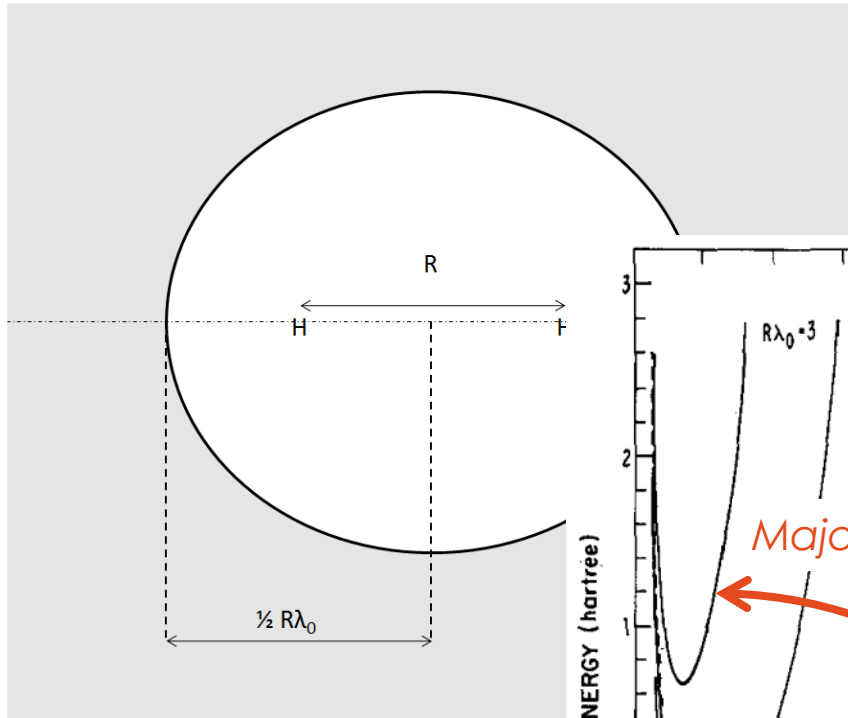


Bond shortening - The physical wall

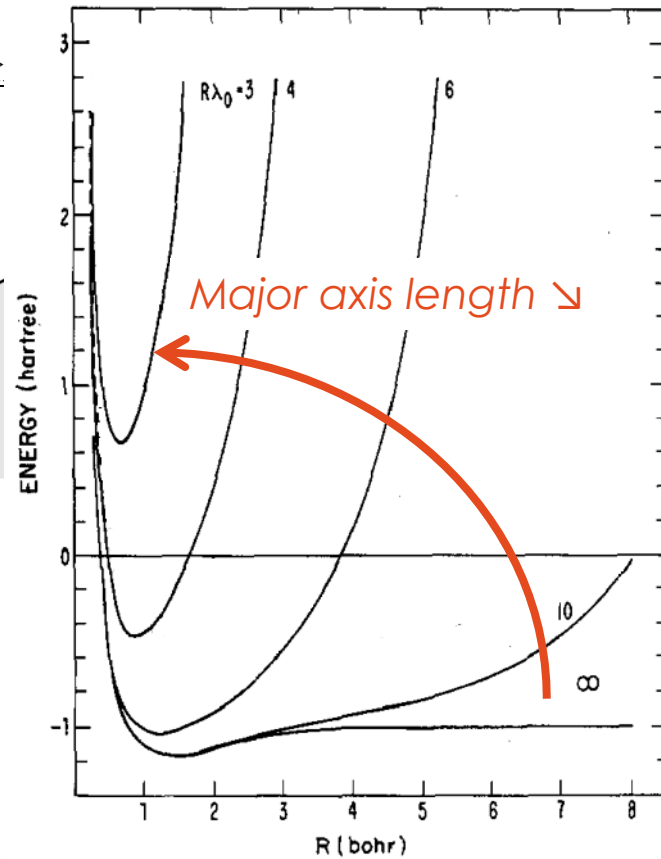


H₂ molecule in a
spheroidal box

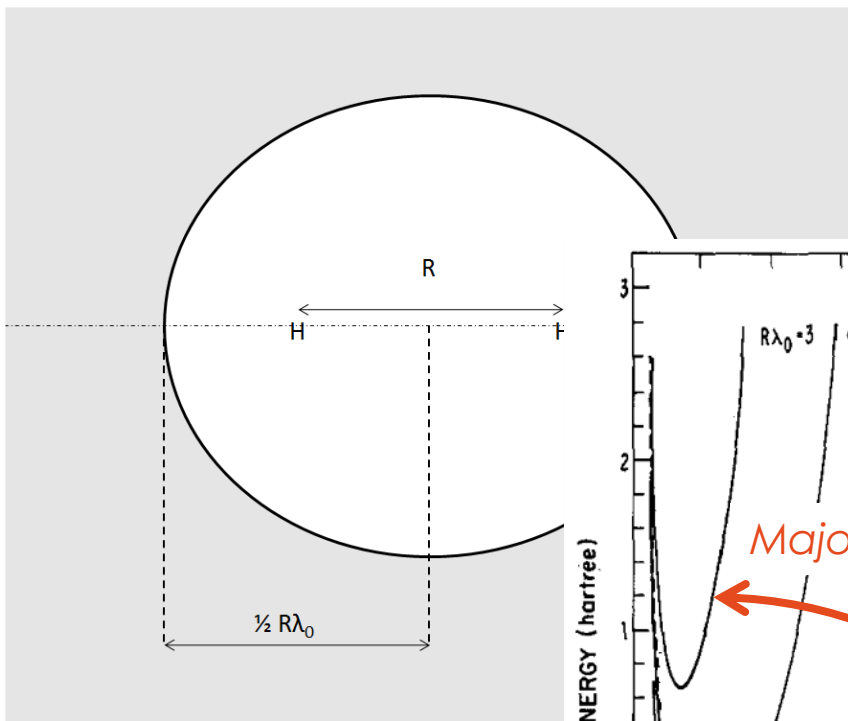
Bond shortening - The physical wall



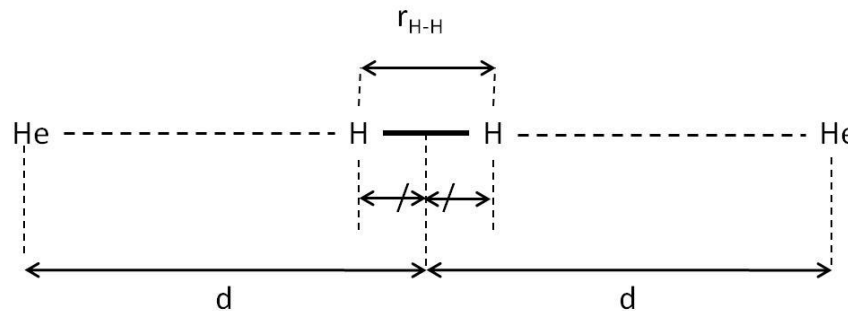
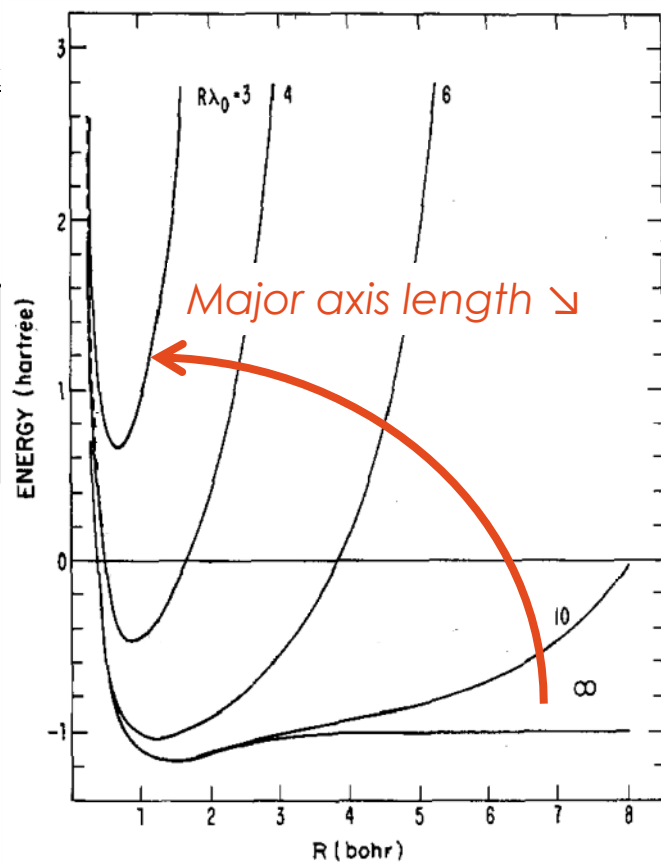
H₂ molecule in a spheroidal box



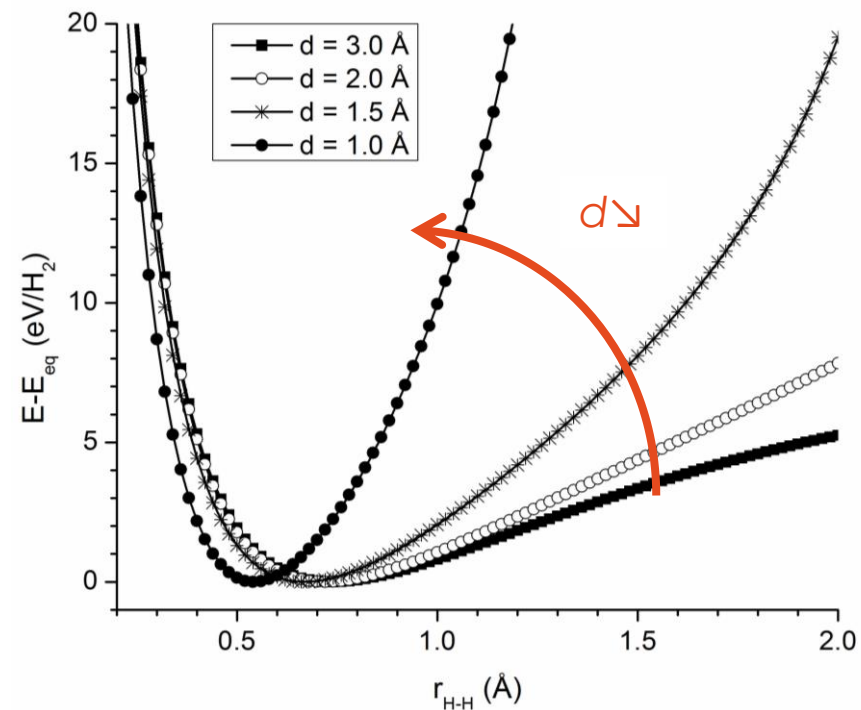
Bond shortening - The physical wall



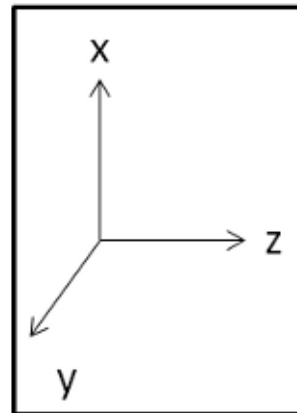
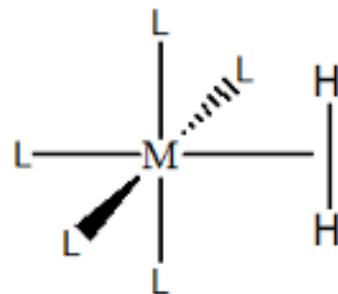
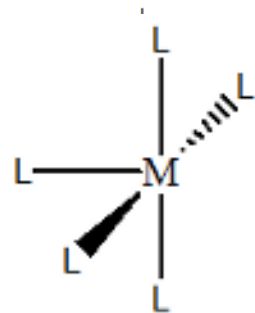
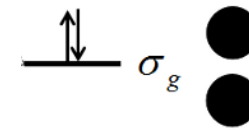
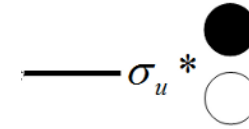
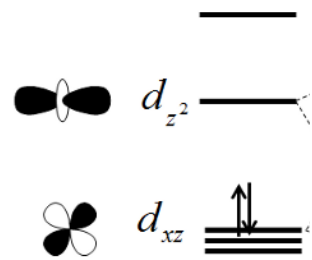
H₂ molecule in a spheroidal box



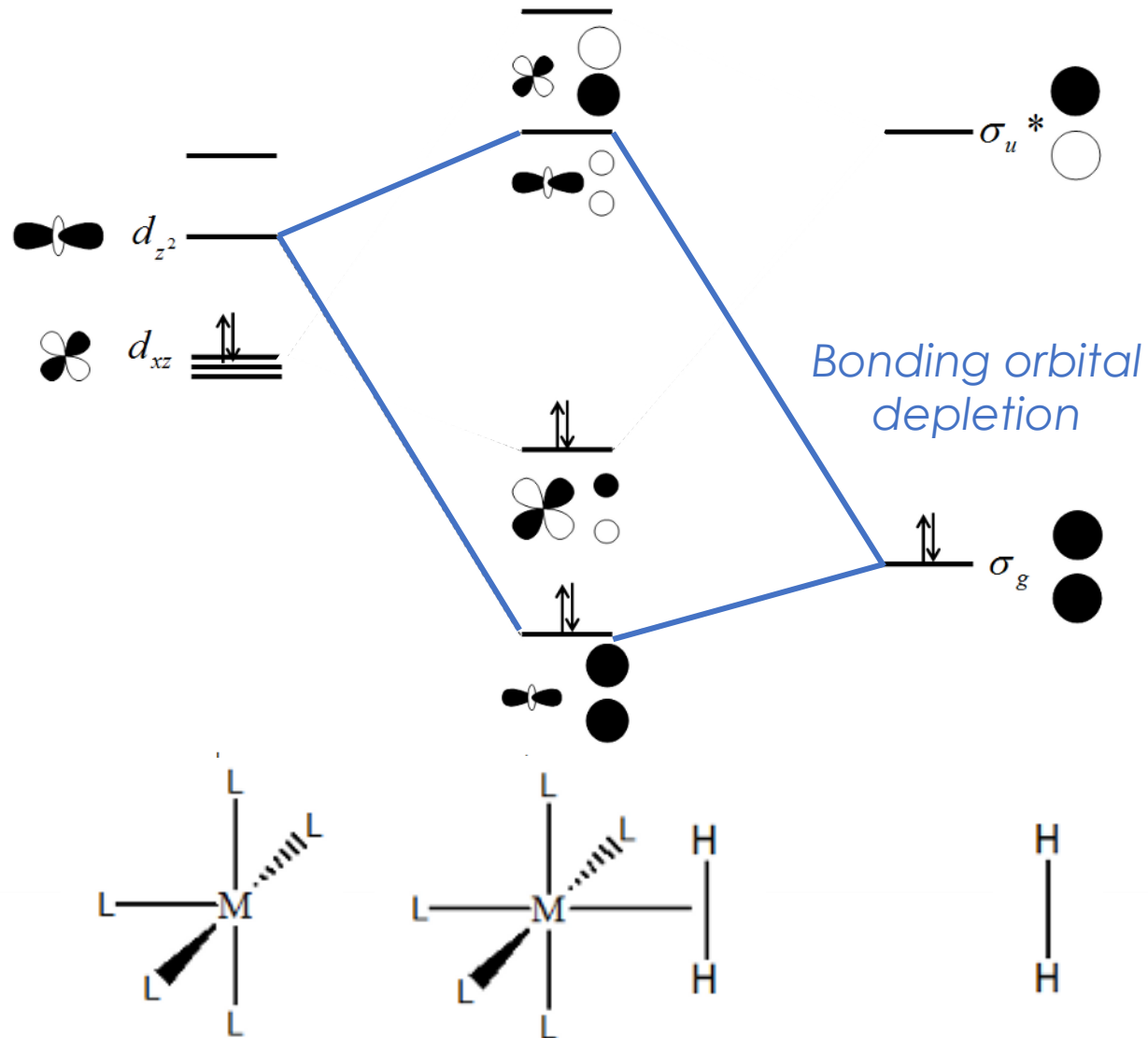
H₂ molecule between 2 He atoms



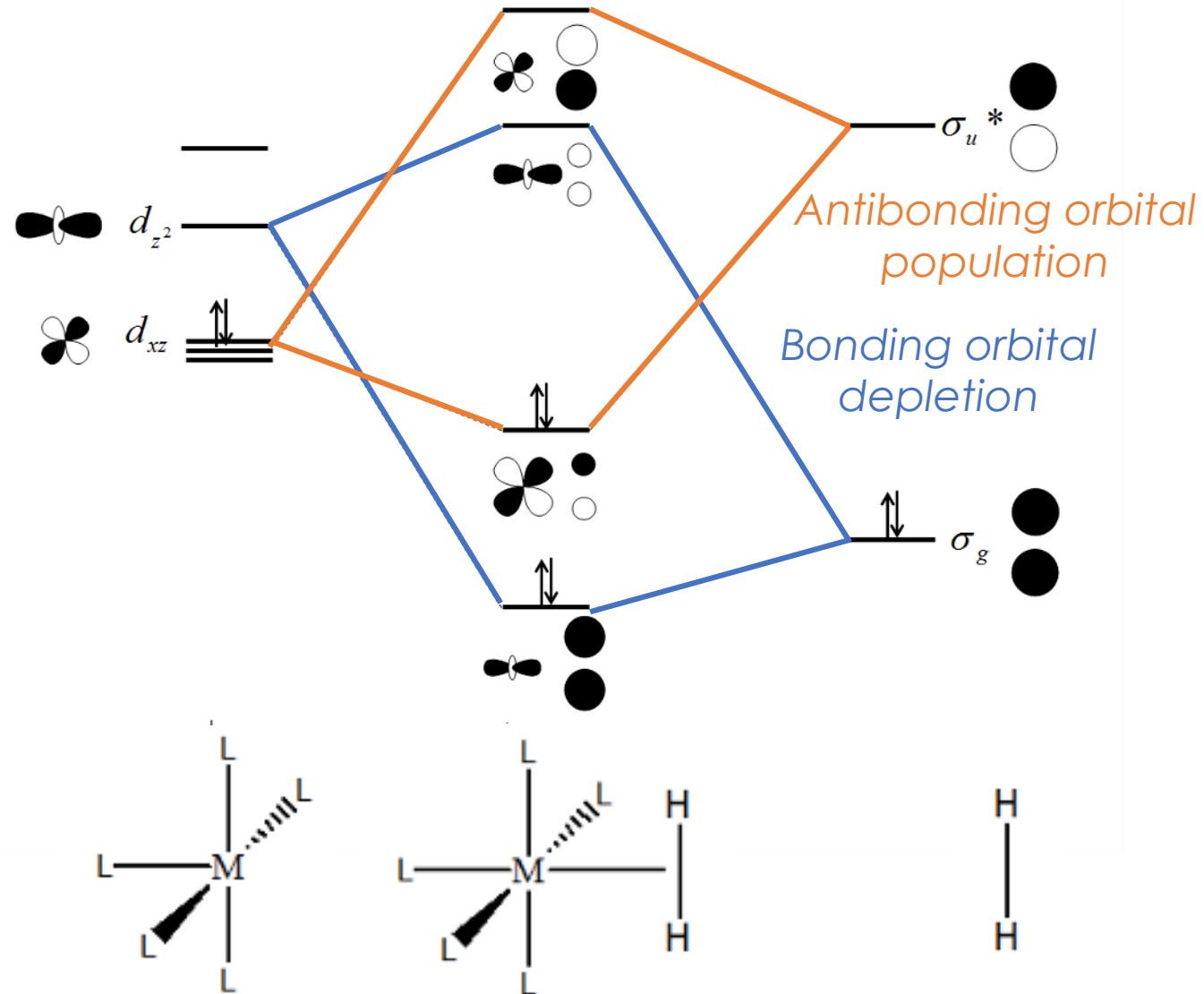
Bond lengthening – Orbital mixing



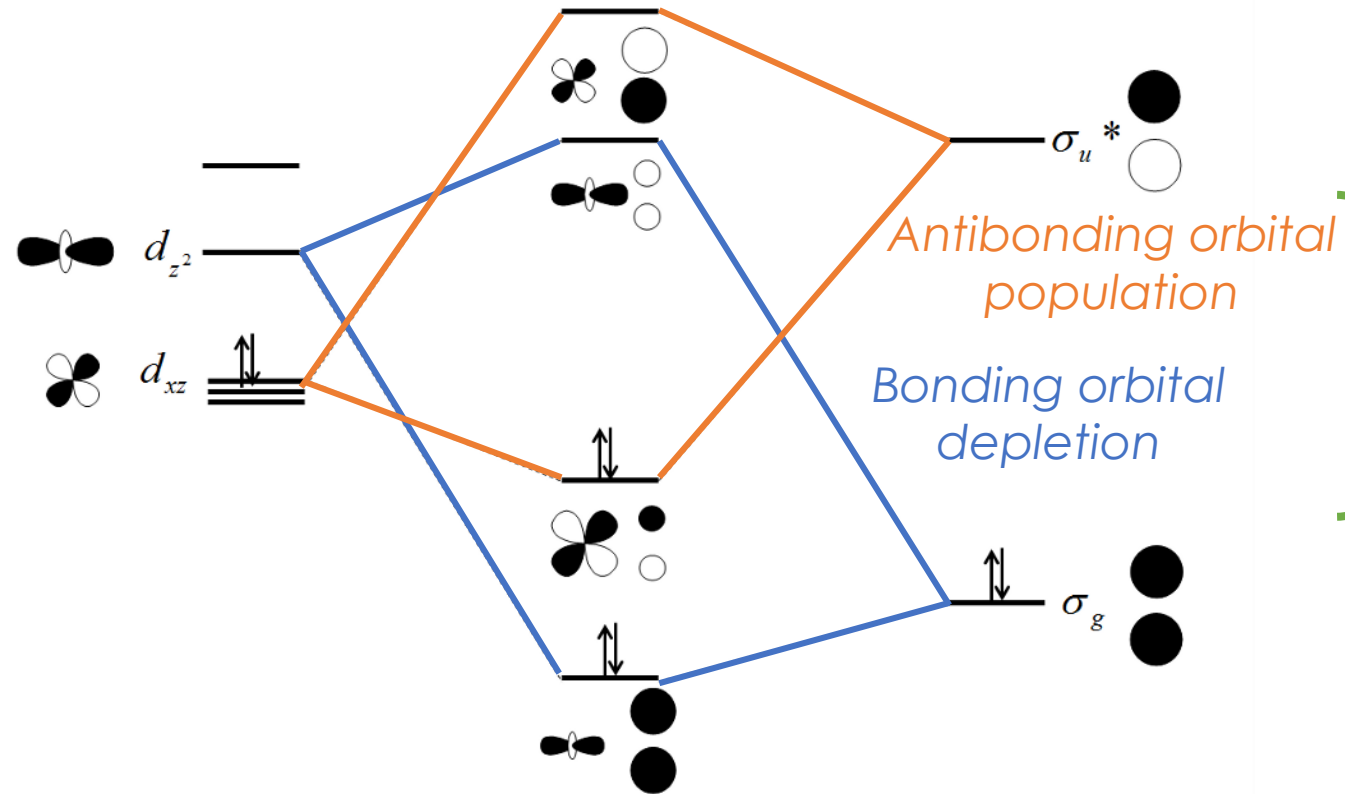
Bond lengthening – Orbital mixing



Bond lengthening – Orbital mixing



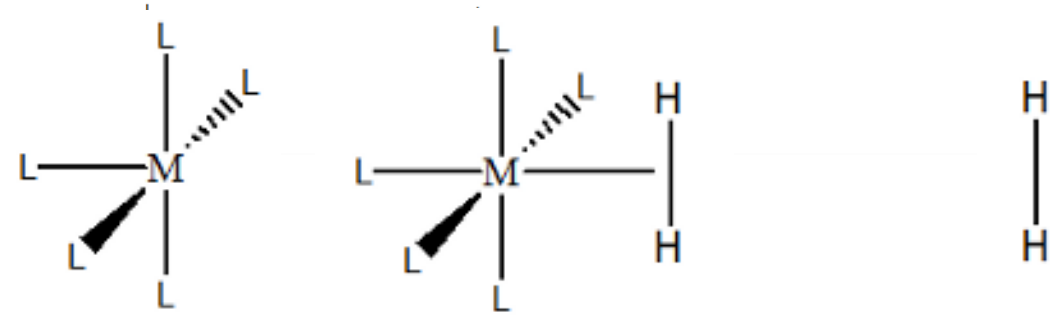
Bond lengthening – Orbital mixing



Kubas complexes

electron transfer from σ_g to σ_u^* via the ML_n fragment

↓
H-H bond elongation



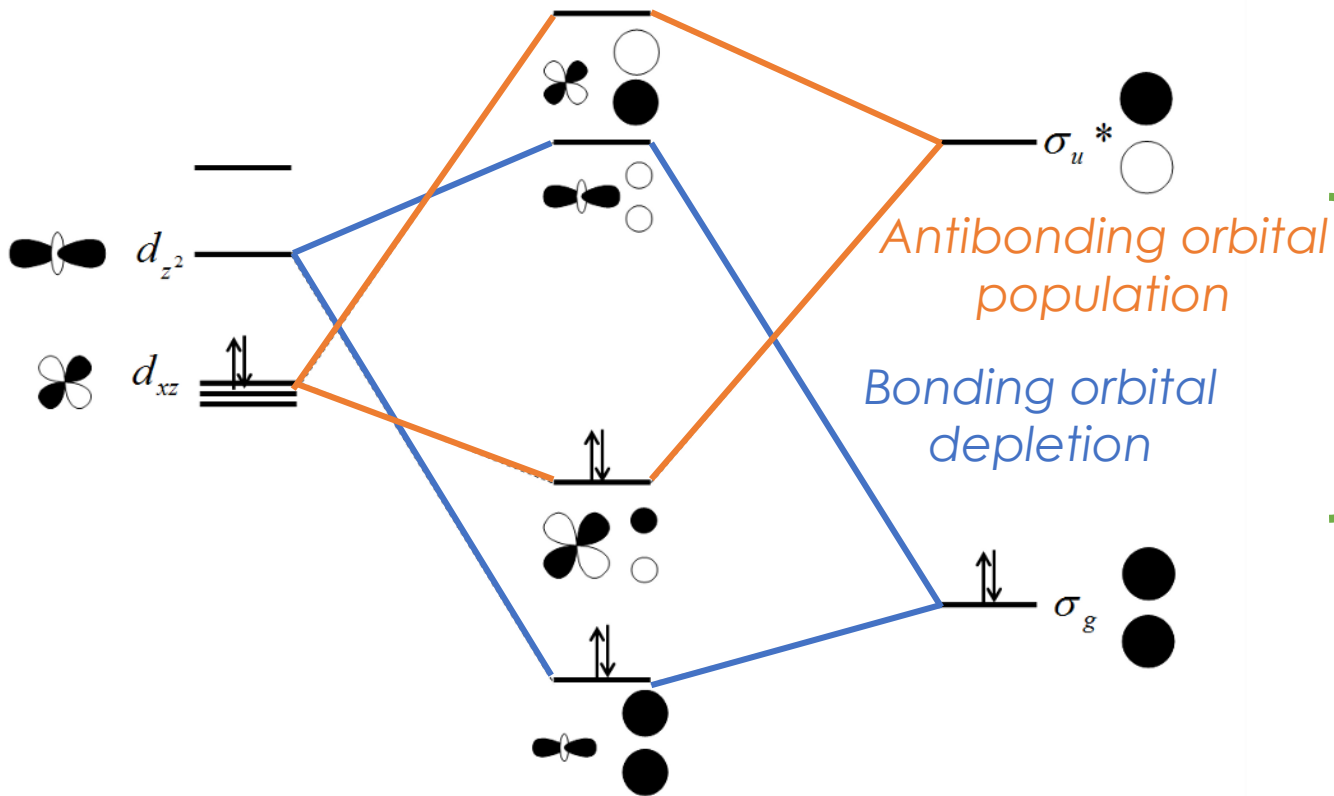
Bond lengthening – Orbital mixing

Solid H under Pressure

electron transfer
from σ_g to σ_u^*

via other H_2 mol.
coming closer and closer

↓
H-H bond
elongation

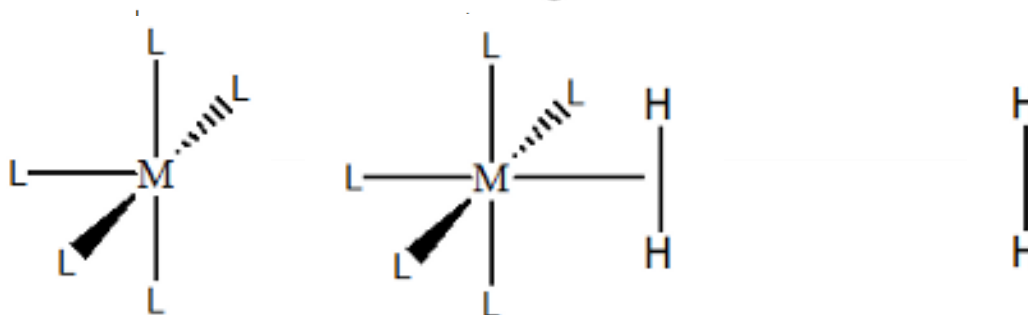


Kubas complexes

electron transfer
from σ_g to σ_u^*

via the ML_n fragment

↓
H-H bond
elongation



Intermediate summary

As P increases

H-H intramolecular bonds

First **strengthen**
and **shorten** ...

« Physical wall »

... then **weaken**
and **elongate**

Orbital mixing

Intermediate summary

As P increases

H-H intramolecular bonds

First **strengthen**
and **shorten** ...

... then **weaken**
and **elongate**

« Physical wall »

Orbital mixing

Shortening and **elongation**
observed numerically
on periodic structural models
for dense solid H

Intermediate summary

As P increases

H-H intramolecular bonds

First **strengthen**
and **shorten** ...

... then **weaken**
and **elongate**

« Physical wall »

Orbital mixing

Shortening and **elongation**
observed numerically
on periodic structural models
for dense solid H

What about **strengthening** and **weakening** ?

Badger's rule
(**bond strength** related to **bond length**)

Intermediate summary

As P increases

H-H intramolecular bonds

First **strengthen**
and **shorten** ...

... then **weaken**
and **elongate**

« Physical wall »

Orbital mixing

Shortening and **elongation**
observed numerically
on periodic structural models
for dense solid H

What about **strengthening** and **weakening** ?

Badger's rule
(**bond strength** related to **bond length**)

Use of **topological tools**

Intermediate summary

As P increases

H-H intramolecular bonds

First **strengthen**
and **shorten** ...

... then **weaken**
and **elongate**

« Physical wall »

Orbital mixing

Shortening and **elongation**
observed numerically
on periodic structural models
for dense solid H

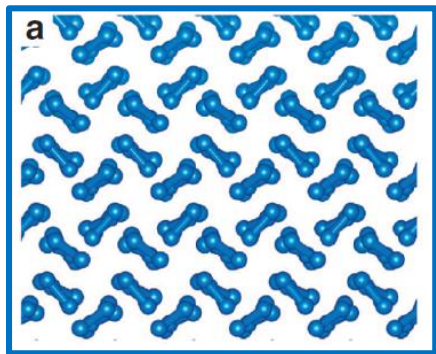
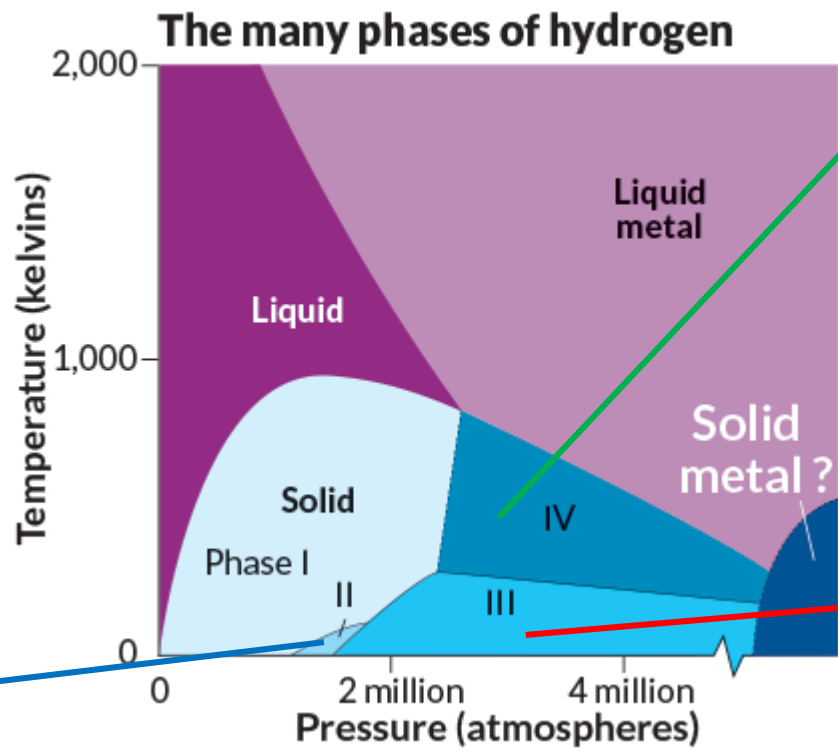
What about **strengthening** and **weakening** ?

Badger's rule
(**bond strength** related to **bond length**)

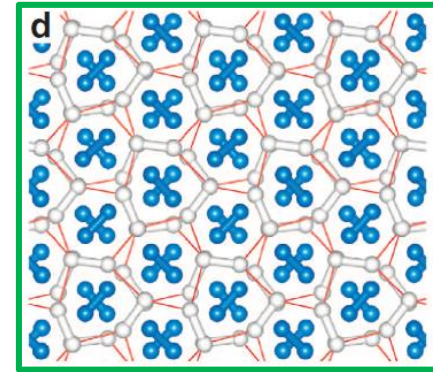
Use of **topological tools**

Relevance of a **cluster model** ?
(easier to manipulate)

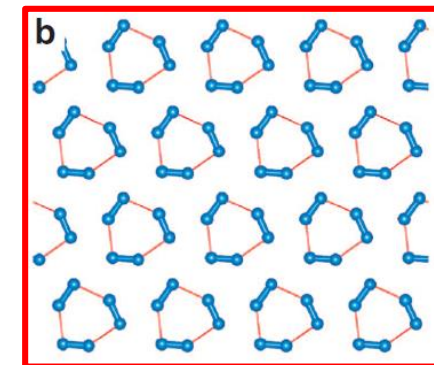
Which structural model for solid H2 under pressure ?



P2₁/c-24 models phase II



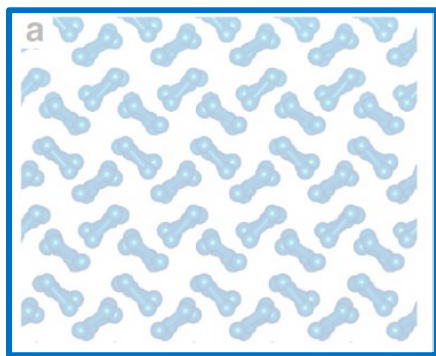
Pc-48 models phase IV



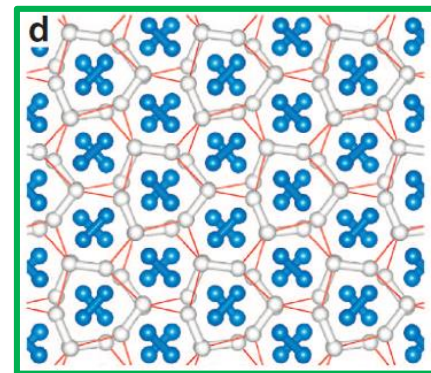
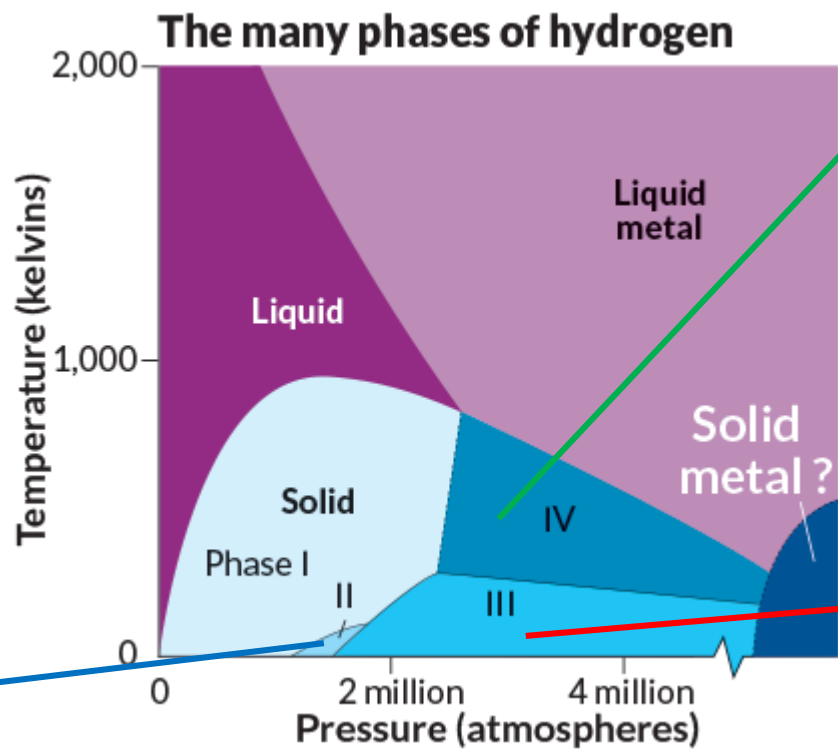
C2/c-24 models phase III

Which structural model for solid H2 under pressure ?

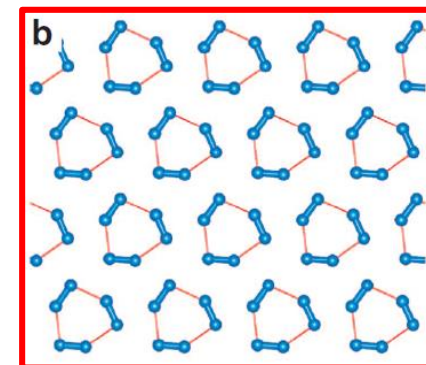
Distorted
graphenelike layers



$P2_1/c-24$ models phase II



Pc-48 models phase IV

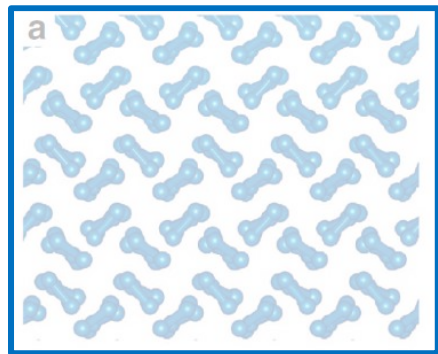


$C2/c-24$ models phase III

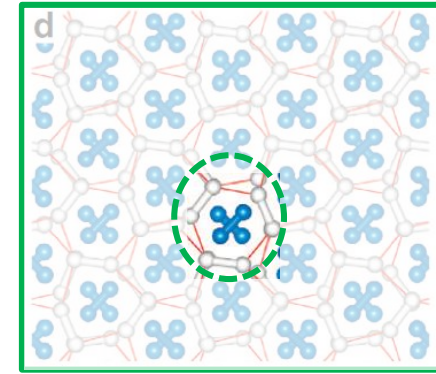
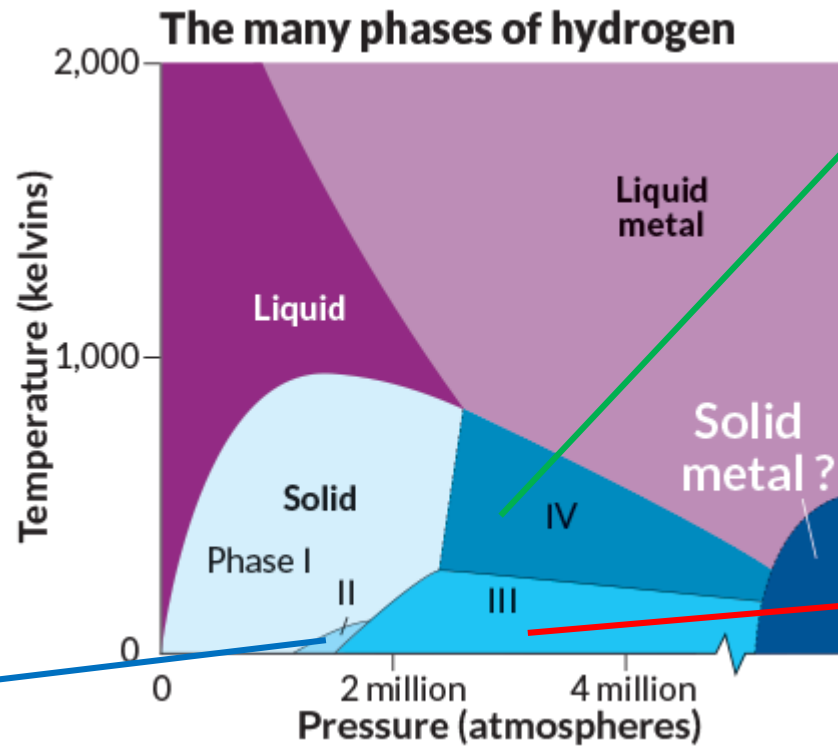
The « 3 H₂ » motif

Distorted
graphenelike layers

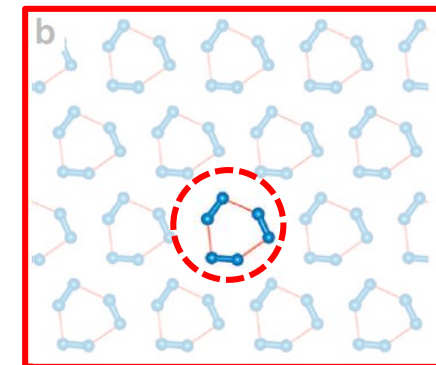
3 H₂ motif



P2₁/c-24 models phase II

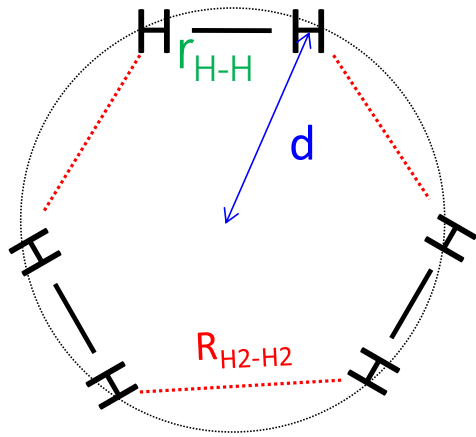


Pc-48 models phase IV

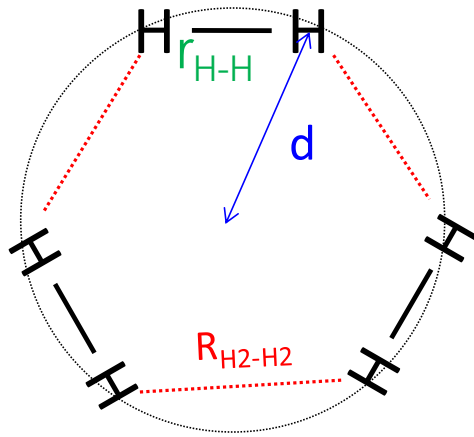


C2/c-24 models phase III

Non-periodic model

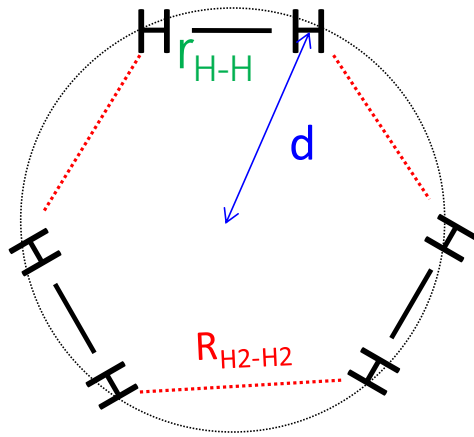


Non-periodic model



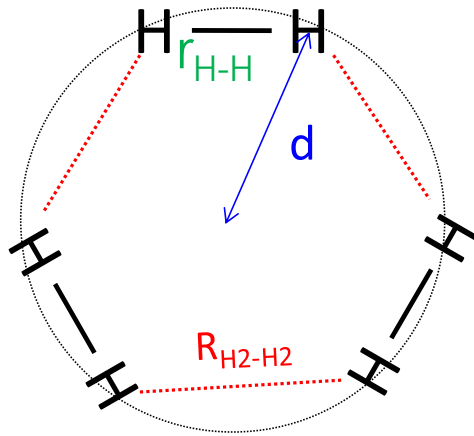
- 6 protons constrained to be on a ring of radius d

Non-periodic model



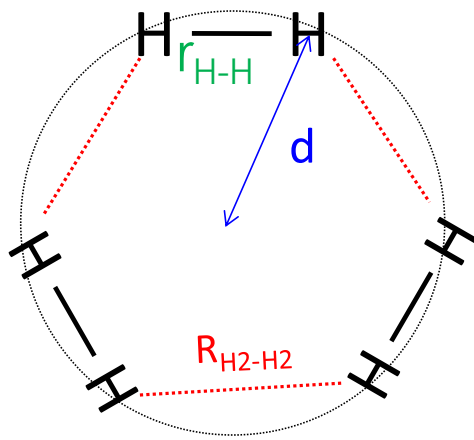
- 6 protons constrained to be on a ring of radius d
- D_{3h} symmetry imposed
→ 1 degree of freedom to optimize $(r_{\text{H-H}}, R_{\text{H2-H2}})$

Non-periodic model

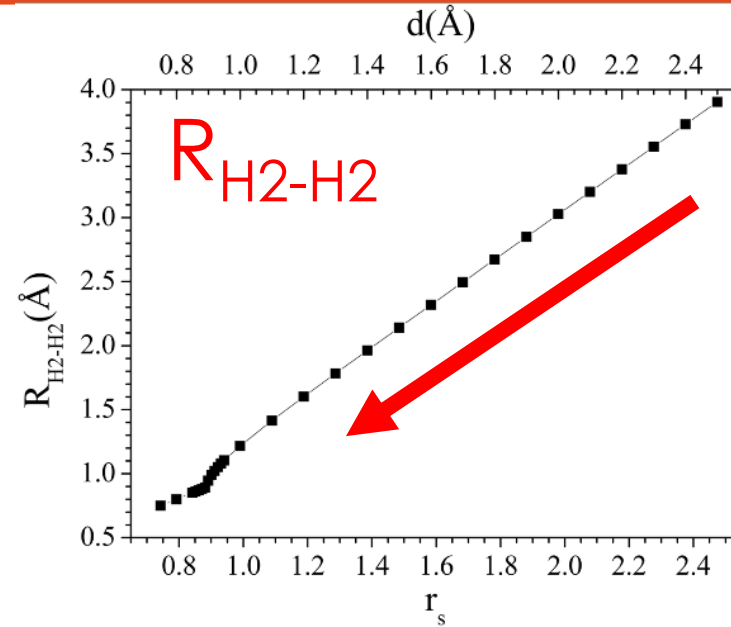


- 6 protons constrained to be on a ring of radius d
- D_{3h} symmetry imposed
→ 1 degree of freedom to optimize ($r_{\text{H-H}}$, $R_{\text{H2-H2}}$)
- d ↘ to model P ↗

Non-periodic model

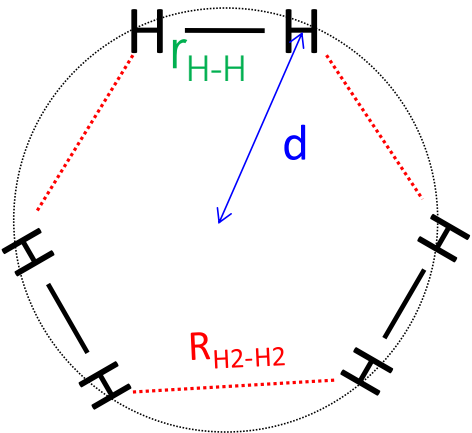


- 6 protons constrained to be on a ring of radius d
- D_{3h} symmetry imposed
→ 1 degree of freedom to optimize ($r_{\text{H-H}}$, $R_{\text{H}_2\text{-H}_2}$)
- $d \searrow$ to model P \nearrow

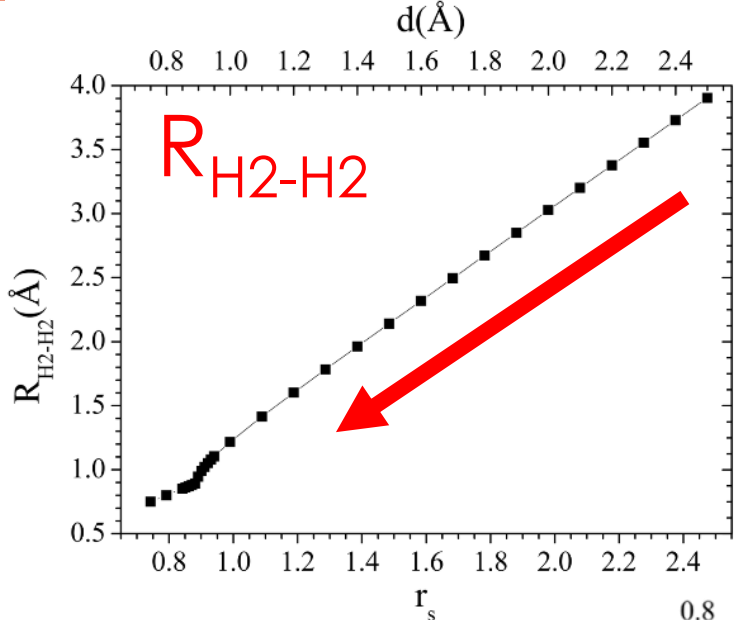


van der Waals space squeezed out

Non-periodic model



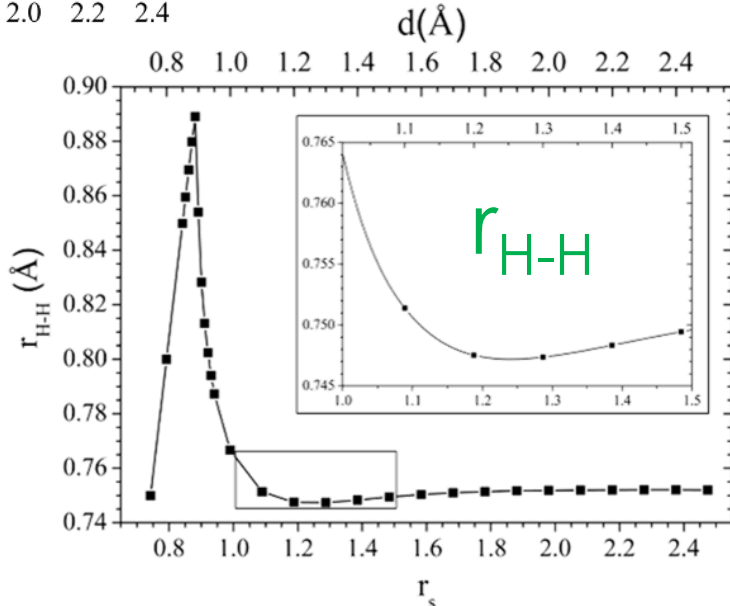
- 6 protons constrained to be on a ring of radius d
- D_{3h} symmetry imposed \rightarrow 1 degree of freedom to optimize (r_{H-H} , $R_{H_2-H_2}$)
- $d \searrow$ to model P \nearrow



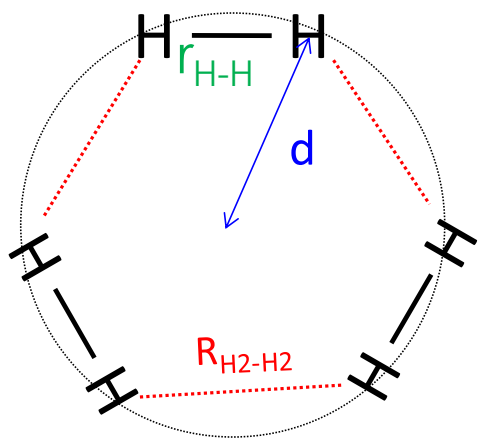
van der Waals space squeezed out

Reproduction of the non monotonous behavior of the H_2 bond length

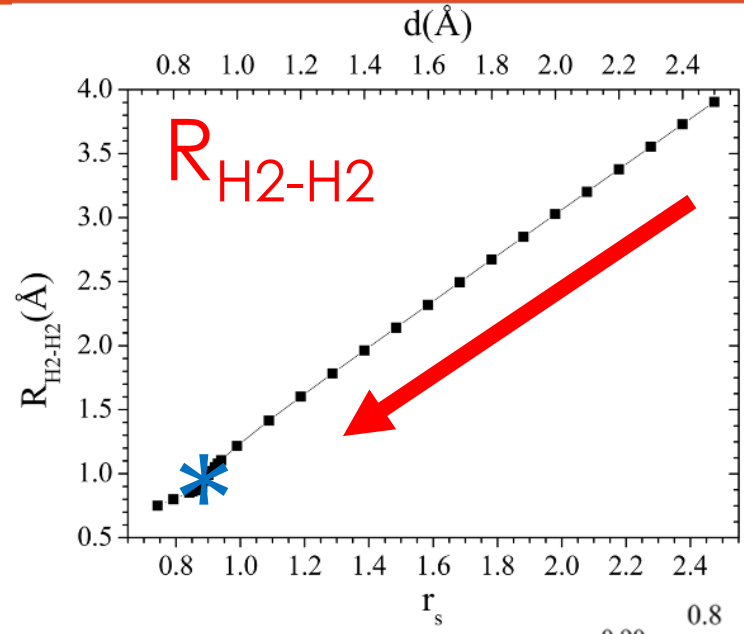
$P \nearrow$ (or $d \searrow$)
 $r_{H-H} \searrow$ then \nearrow then \searrow



Non-periodic model



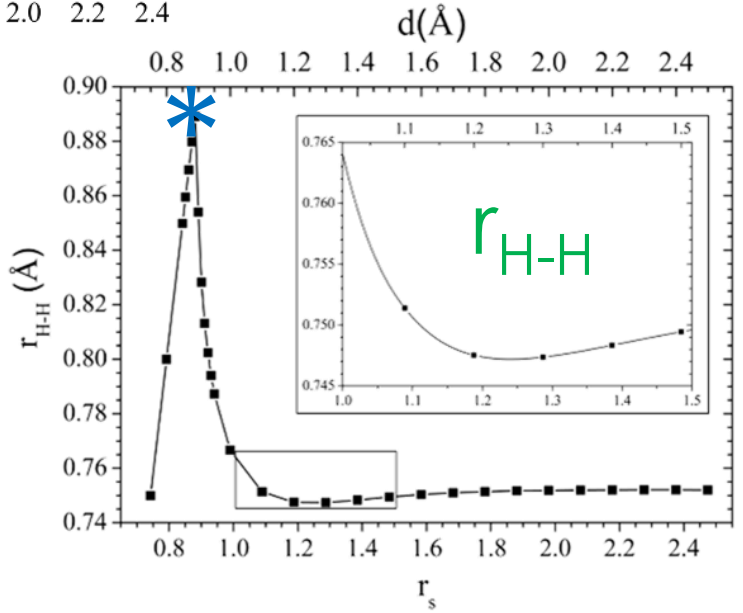
- 6 protons constrained to be on a ring of radius d
- D_{3h} symmetry imposed \rightarrow 1 degree of freedom to optimize (r_{H-H} , R_{H2-H2})
- $d \searrow$ to model P \nearrow



van der Waals space squeezed out

Reproduction of the non monotonous behavior of the H_2 bond length

$P \nearrow$ (or $d \searrow$)
 $r_{H-H} \searrow$ then \nearrow then \searrow



Plotting $s = f(\rho)$

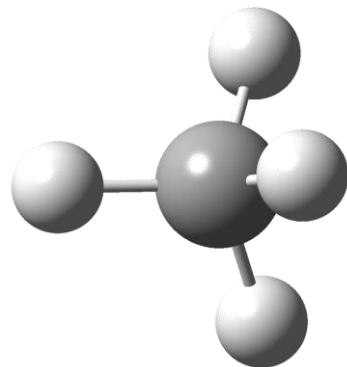
$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

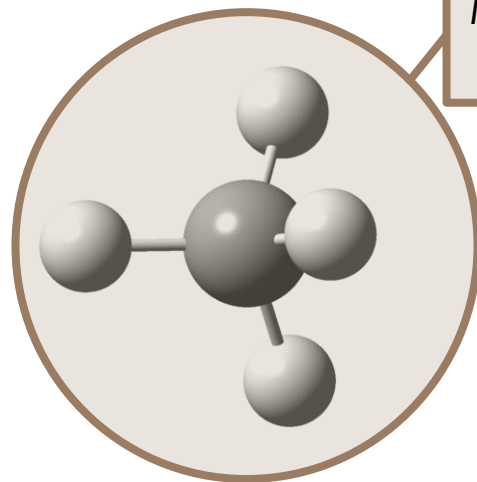


Plotting $s = f(\rho)$

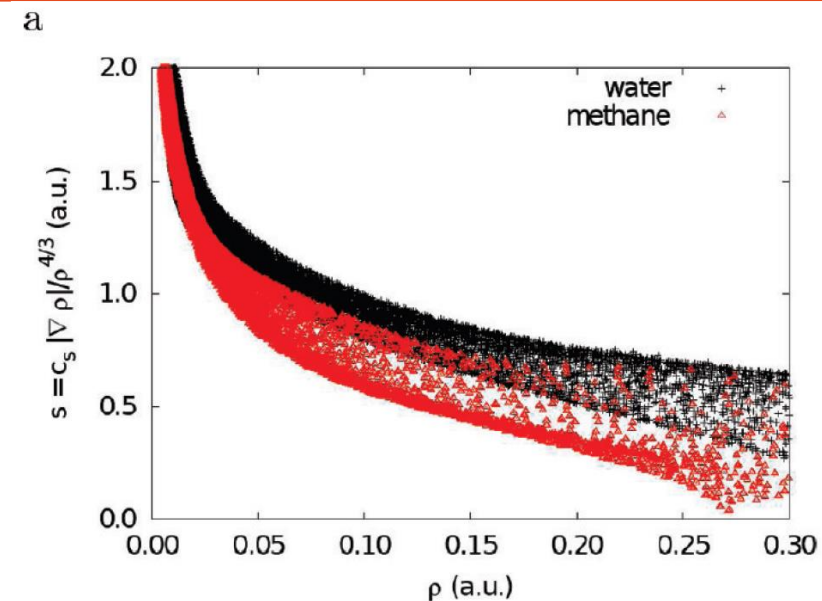
$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

Density tail
Low ρ , high s



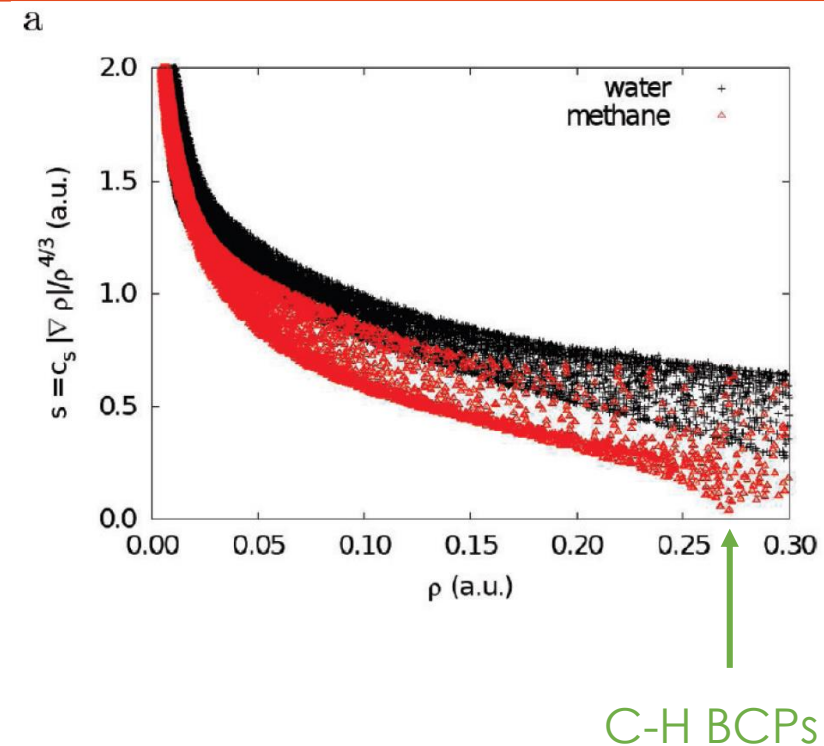
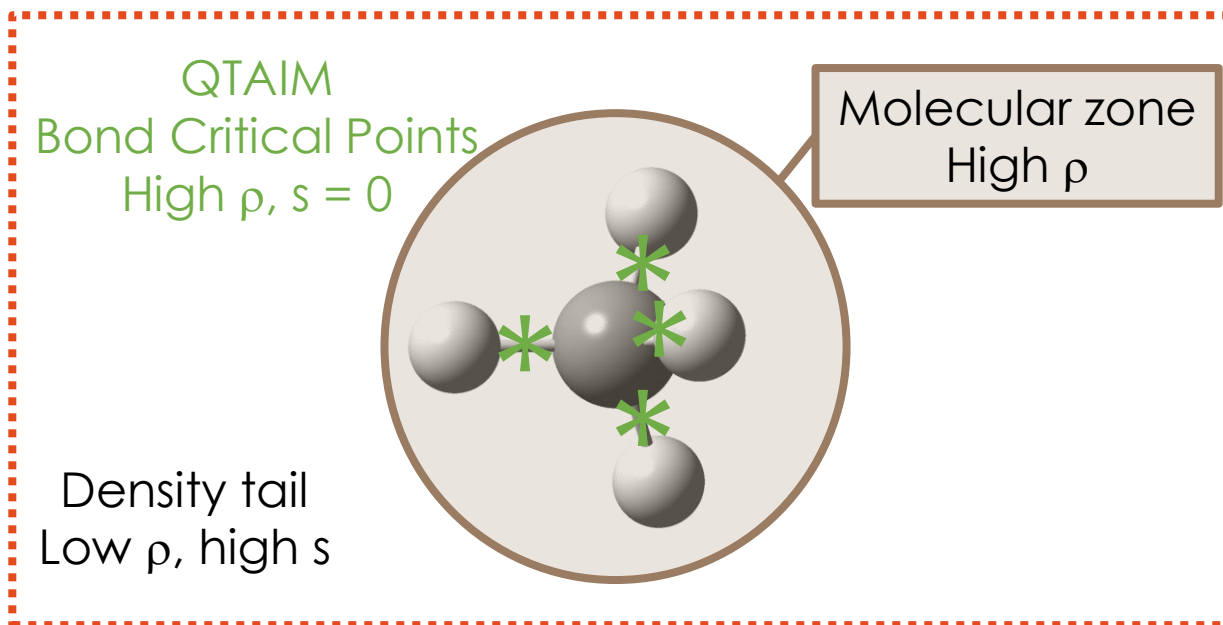
Molecular zone
High ρ



Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

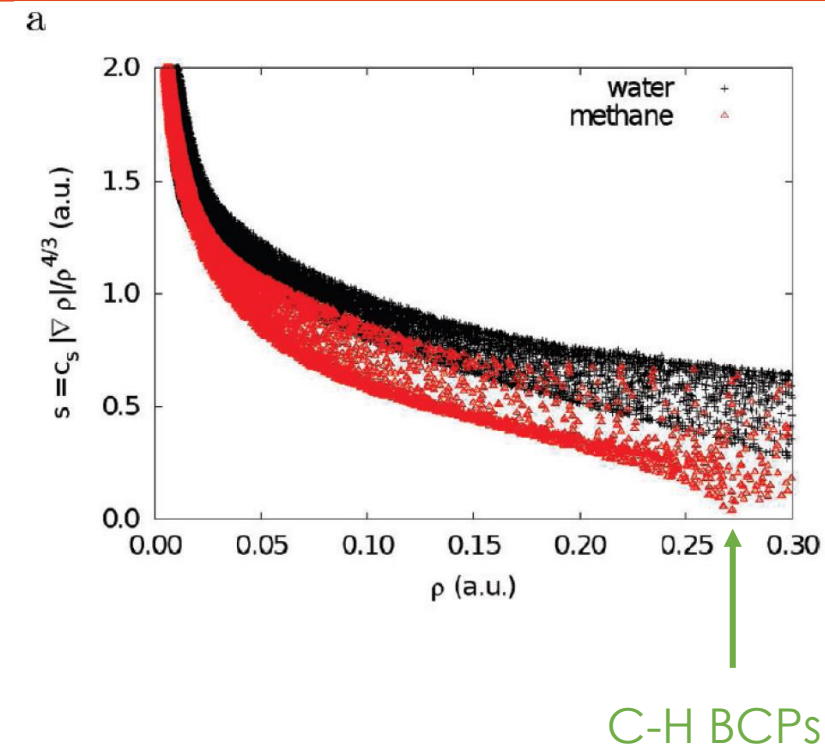
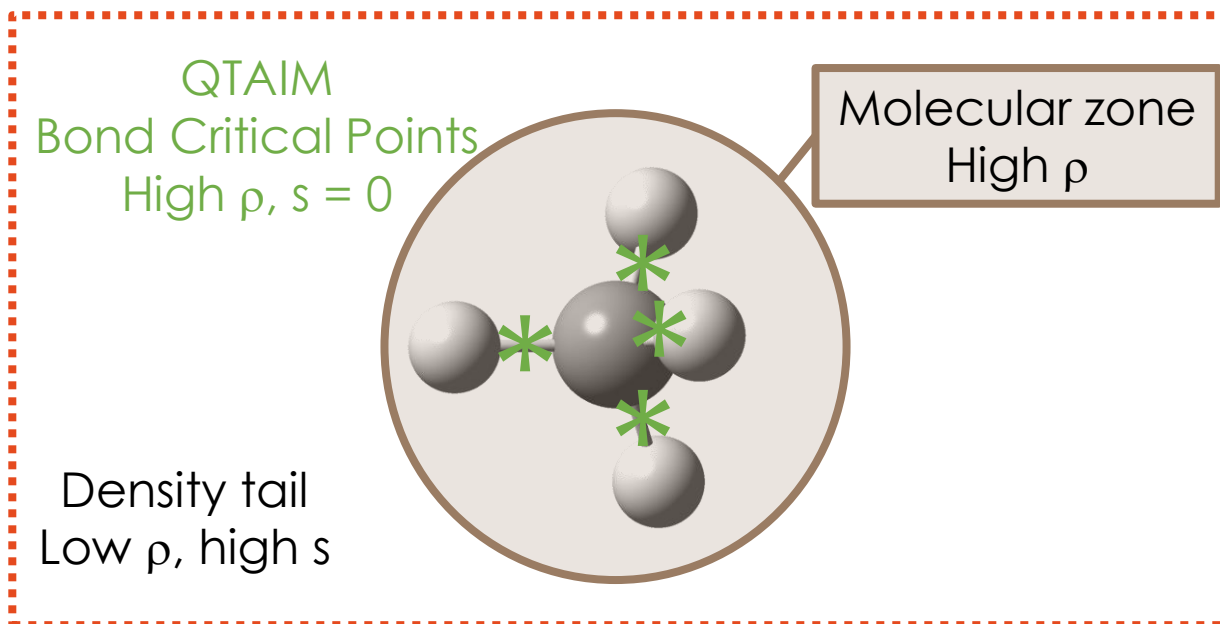


NCI index

Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

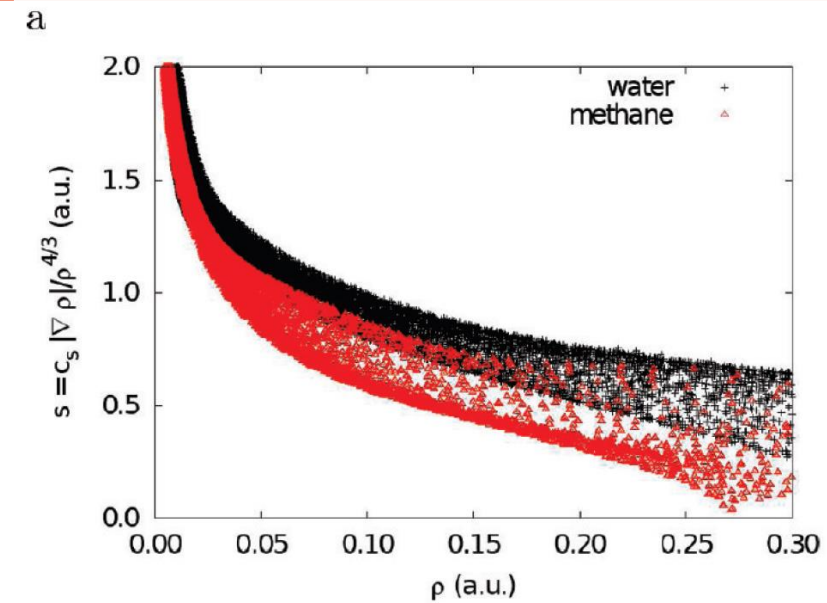
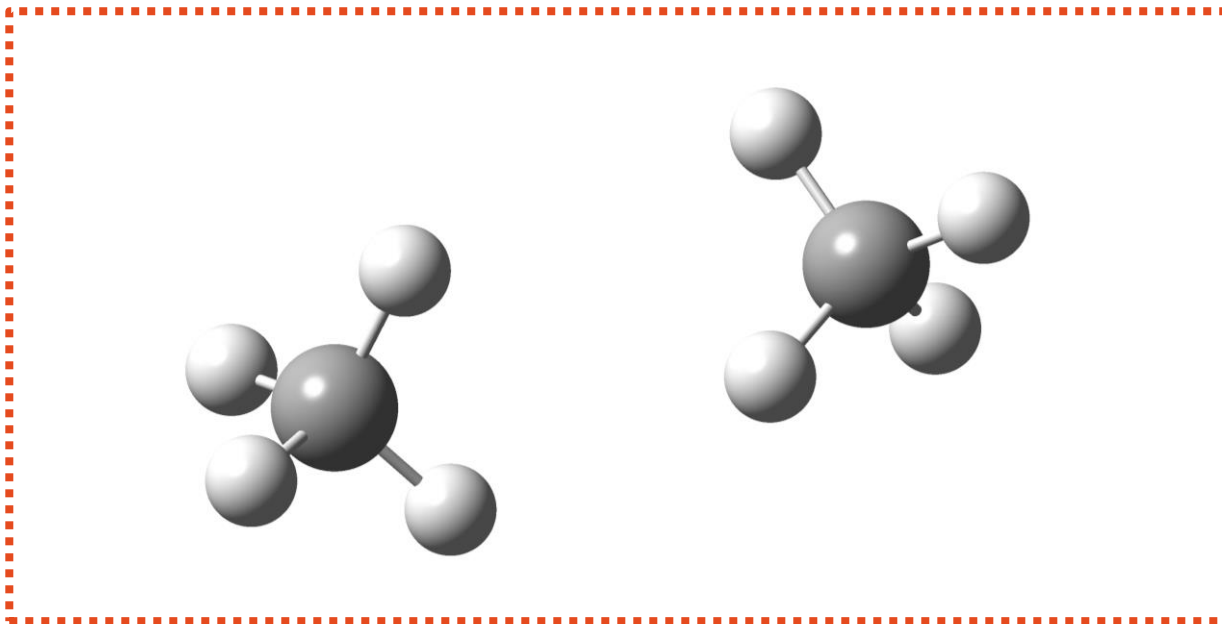


Reveals the presence of
intramolecular interactions

Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

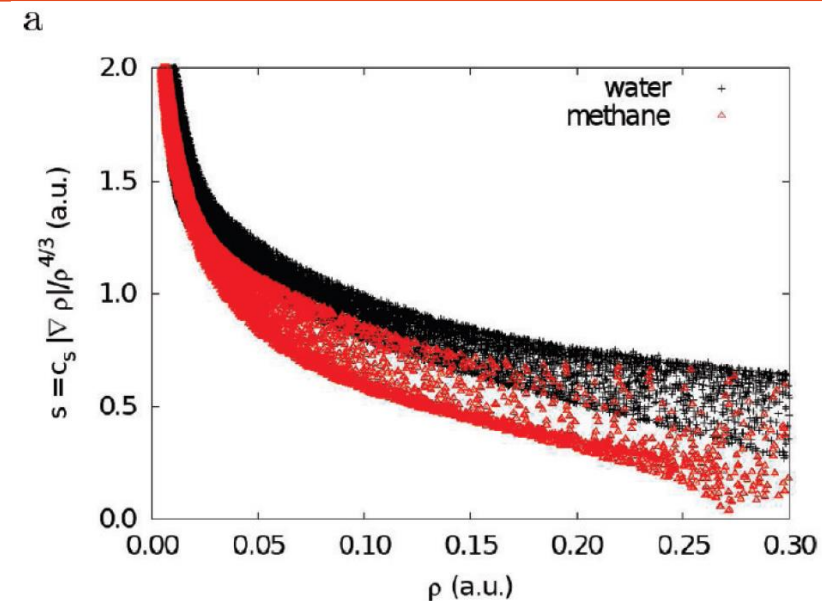
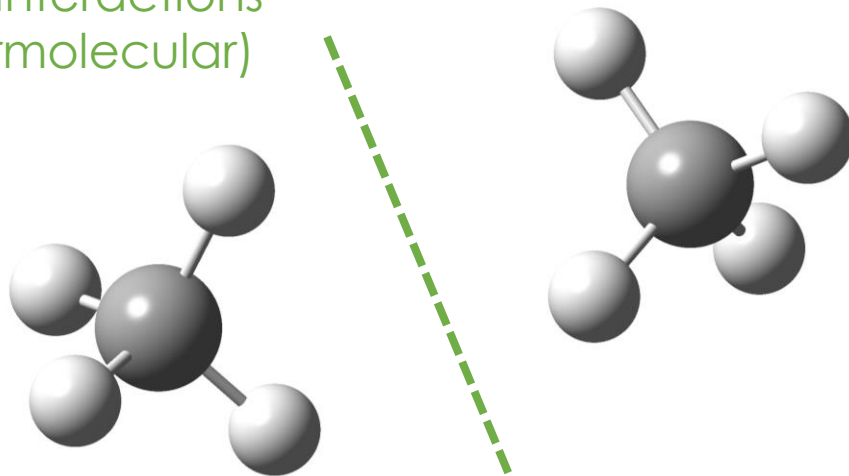


Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

vdW interactions
(intermolecular)

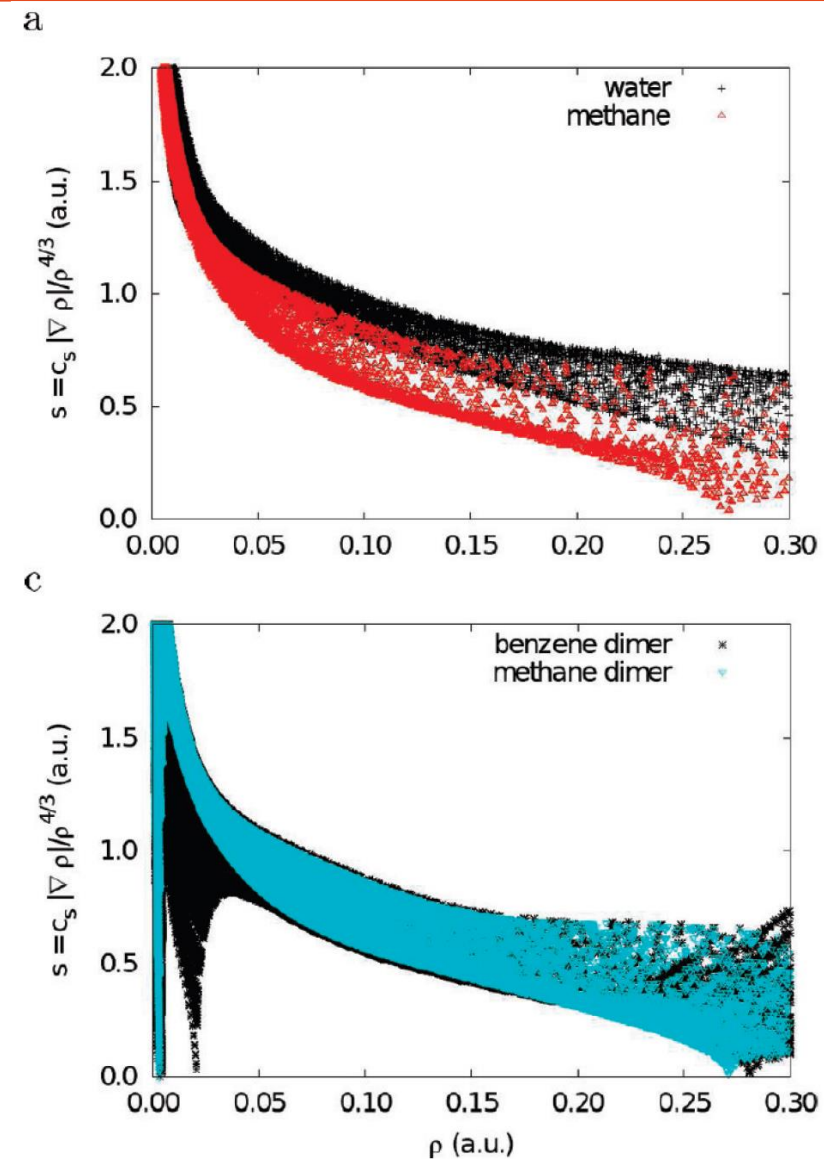
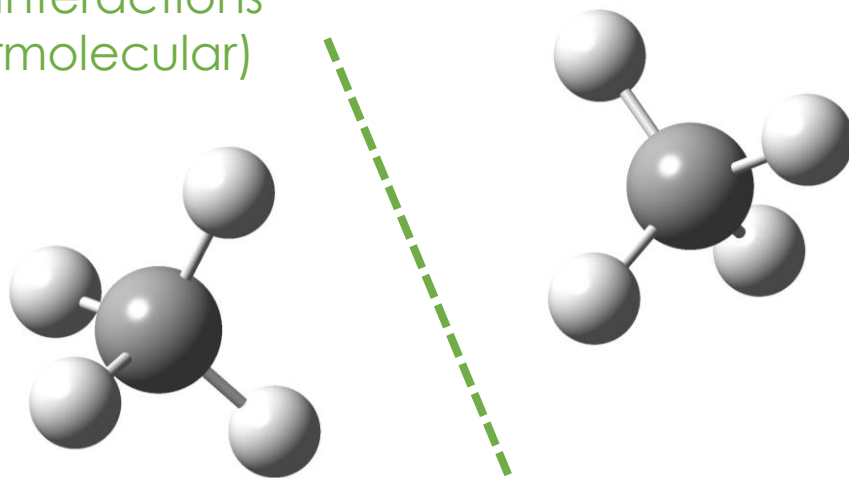


Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

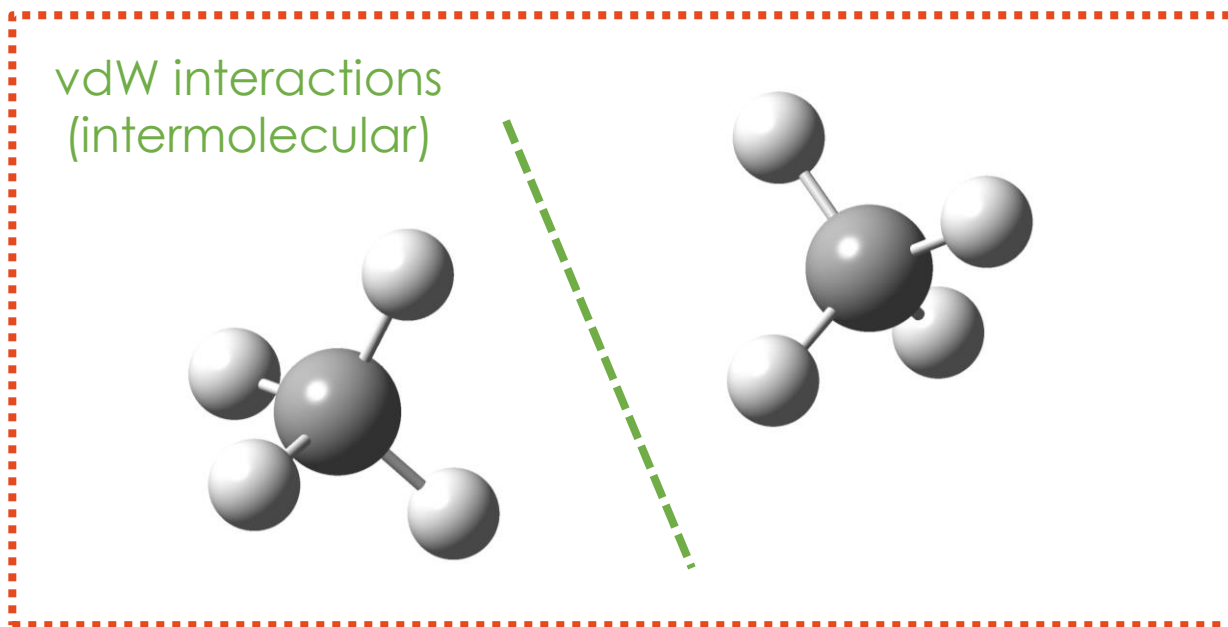
vdW interactions
(intermolecular)



Plotting $s = f(\rho)$

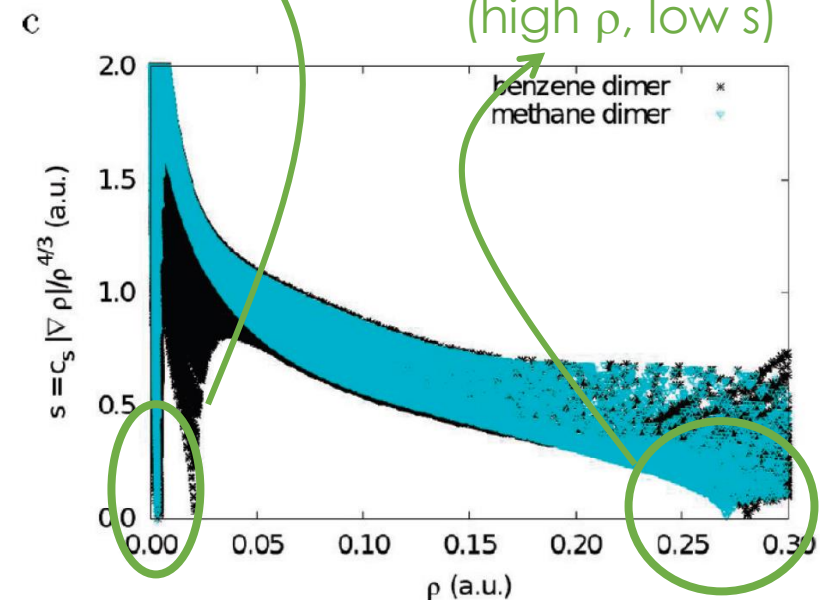
$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density



Intermolecular Interactions (low ρ , low s)

Intramolecular Interactions (high ρ , low s)



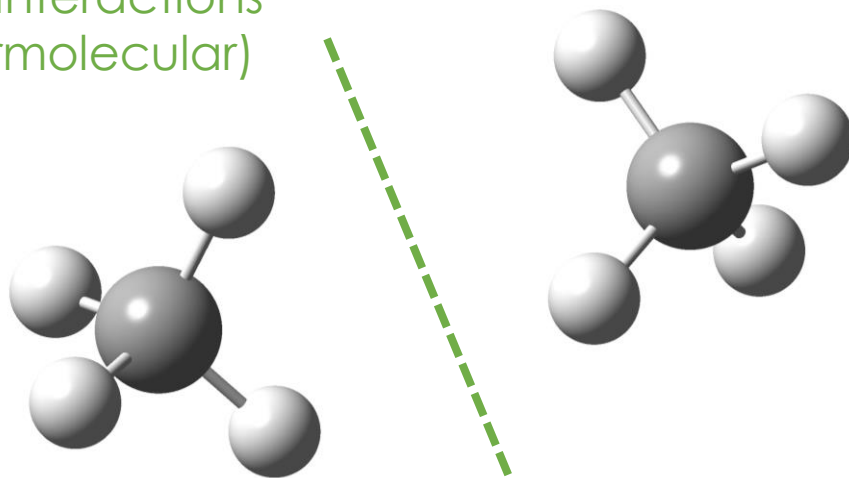
NCI index

Plotting $s = f(\rho)$

$$s = \frac{1}{C_S} \frac{|\nabla\rho|}{\rho^{4/3}}$$

Reduced gradient density

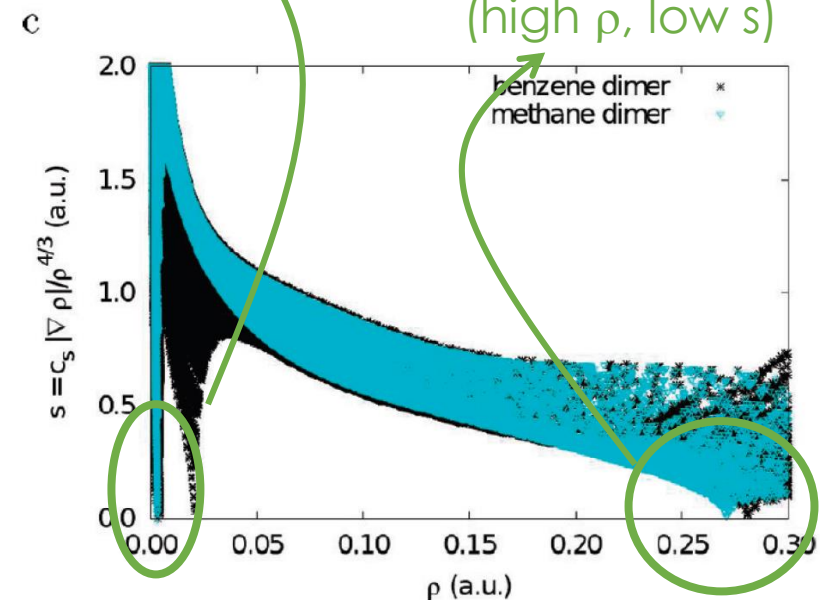
vdW interactions
(intermolecular)



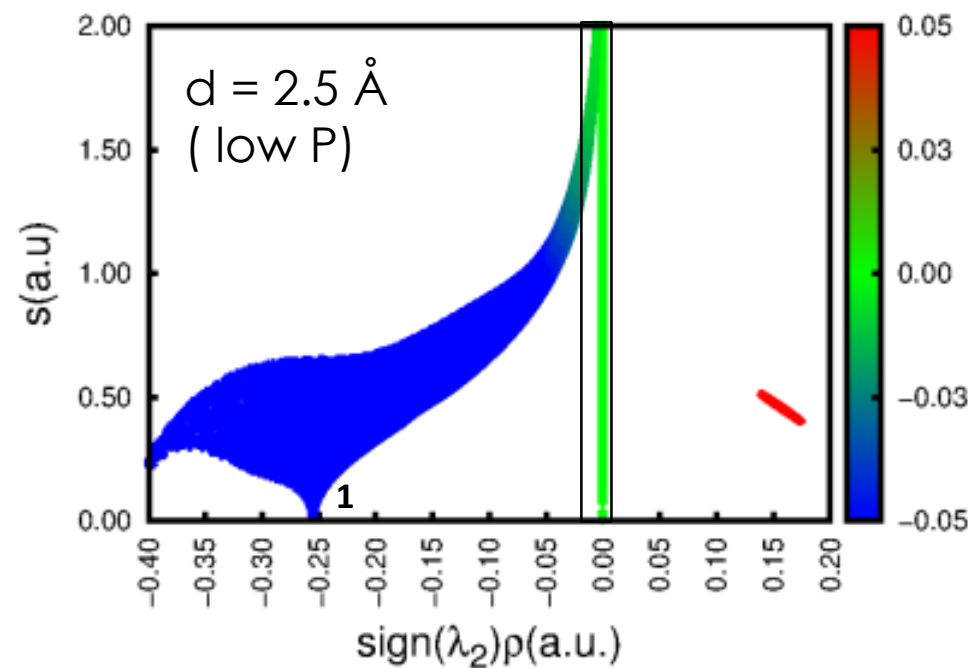
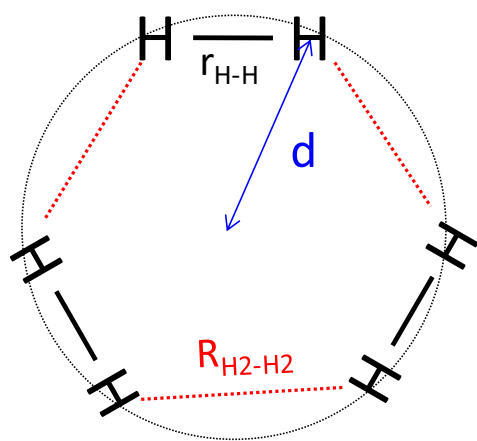
Spikes $\rho \leftrightarrow$ interaction strength

Intermolecular
Interactions
(low ρ , low s)

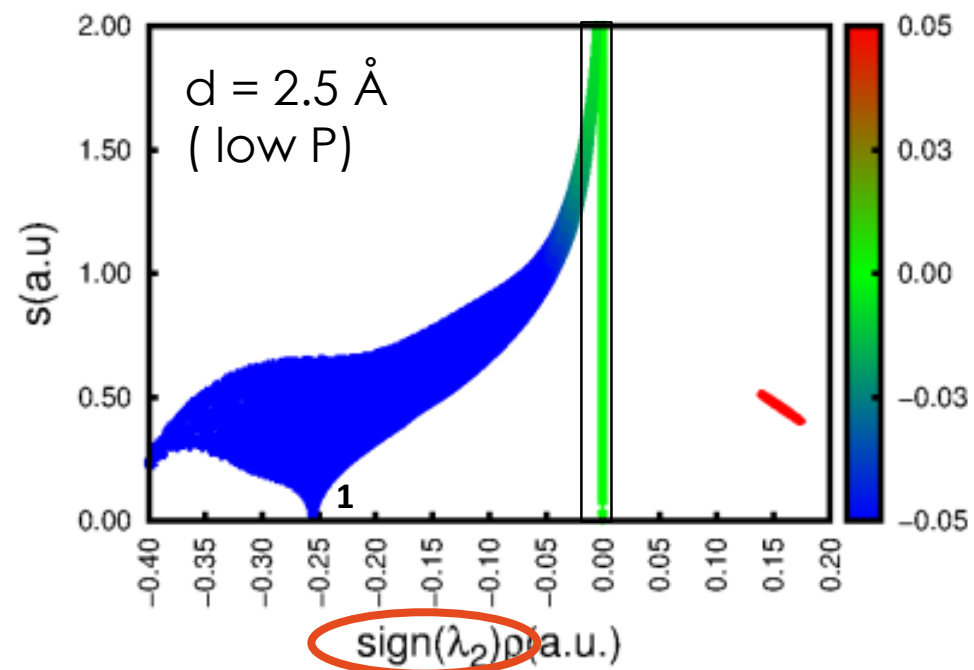
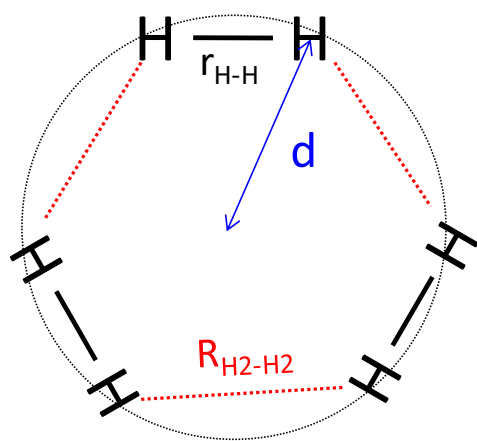
Intramolecular
Interactions
(high ρ , low s)



NCI index – inventaire of the interactions

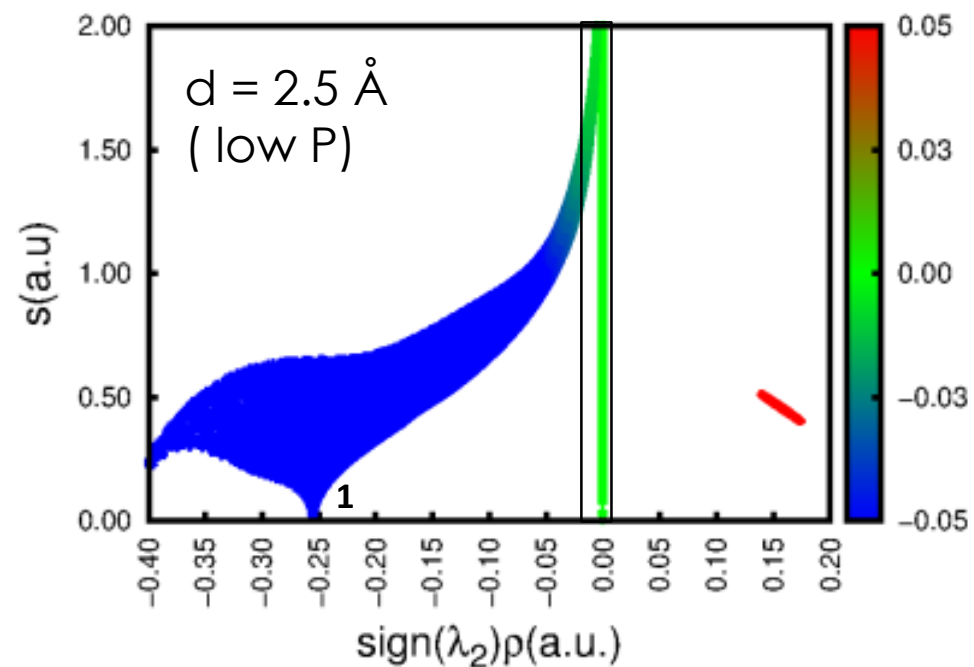
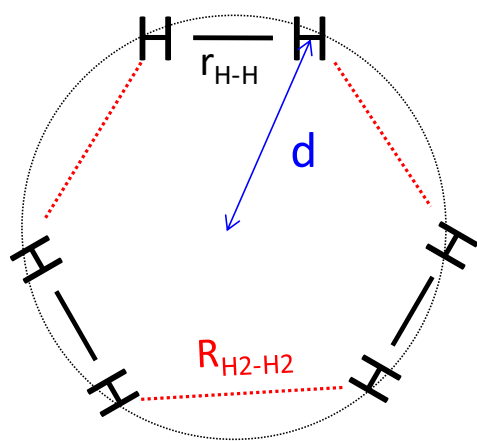


NCI index – inventaire of the interactions



λ_2 : eigenvalue of the ρ Hessian matrix
($\lambda_1 < \lambda_2 < \lambda_3$)

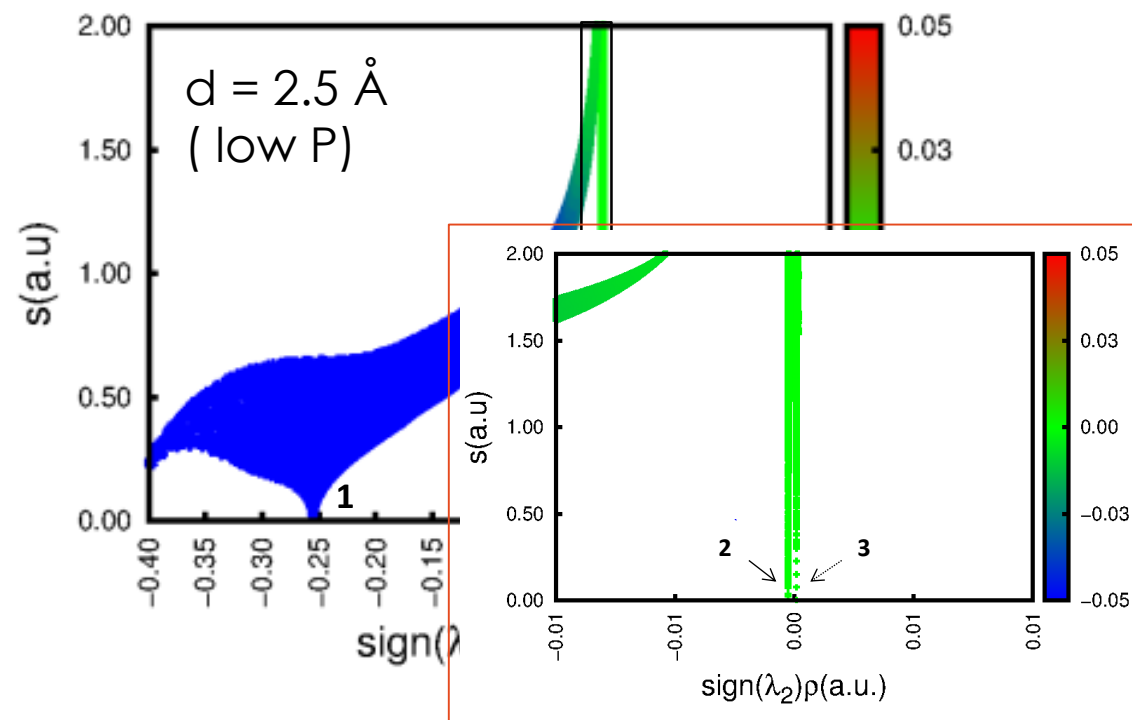
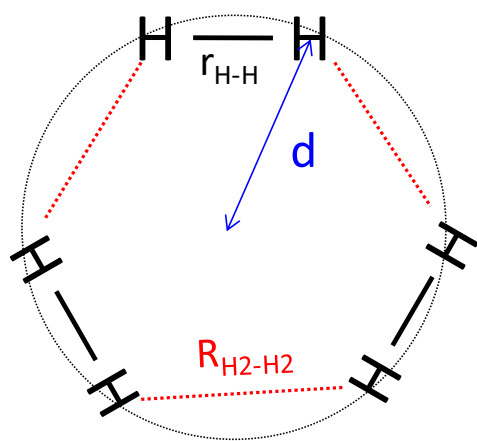
NCI index – inventaire of the interactions



λ_2 : eigenvalue of the ρ Hessian matrix
($\lambda_1 < \lambda_2 < \lambda_3$)

$\lambda_2 < 0$: attractive interaction
 $\lambda_2 > 0$: repulsive interaction

NCI index – inventaire of the interactions

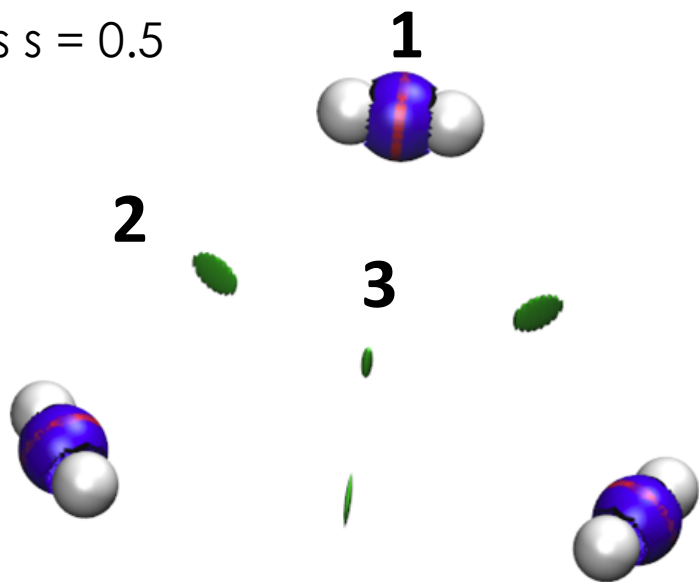


λ_2 : eigenvalue of the ρ Hessian matrix
($\lambda_1 < \lambda_2 < \lambda_3$)

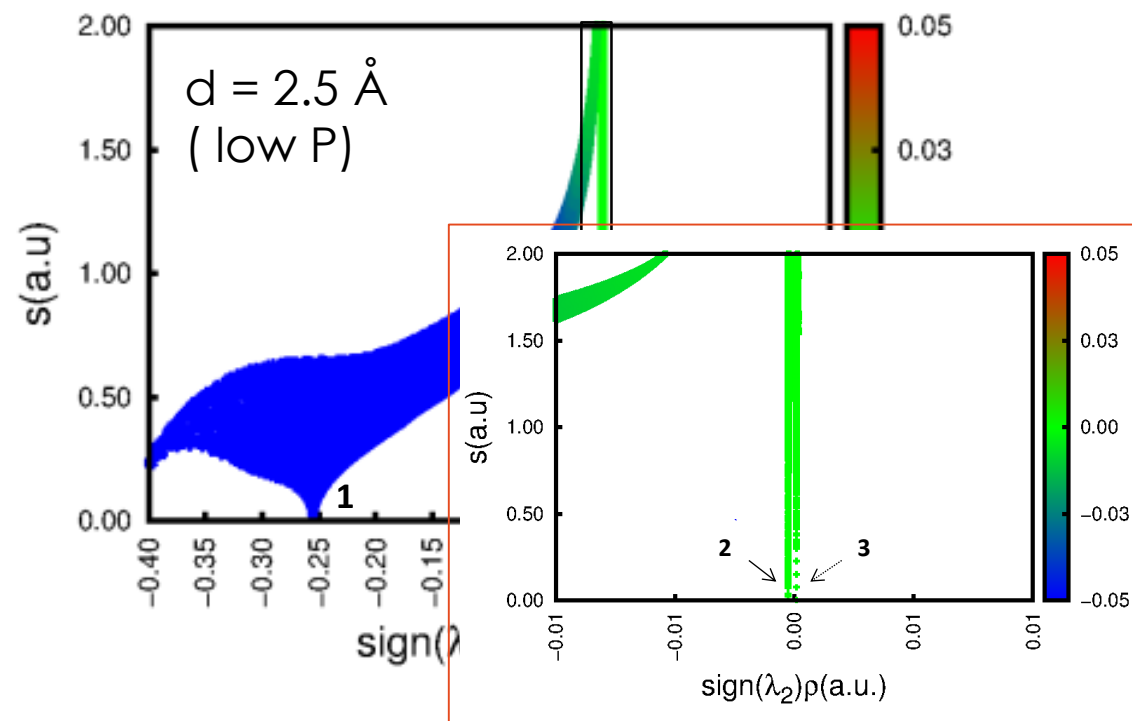
$\lambda_2 < 0$: attractive interaction
 $\lambda_2 > 0$: repulsive interaction

NCI index – inventaire of the interactions

Isosurfaces $s = 0.5$



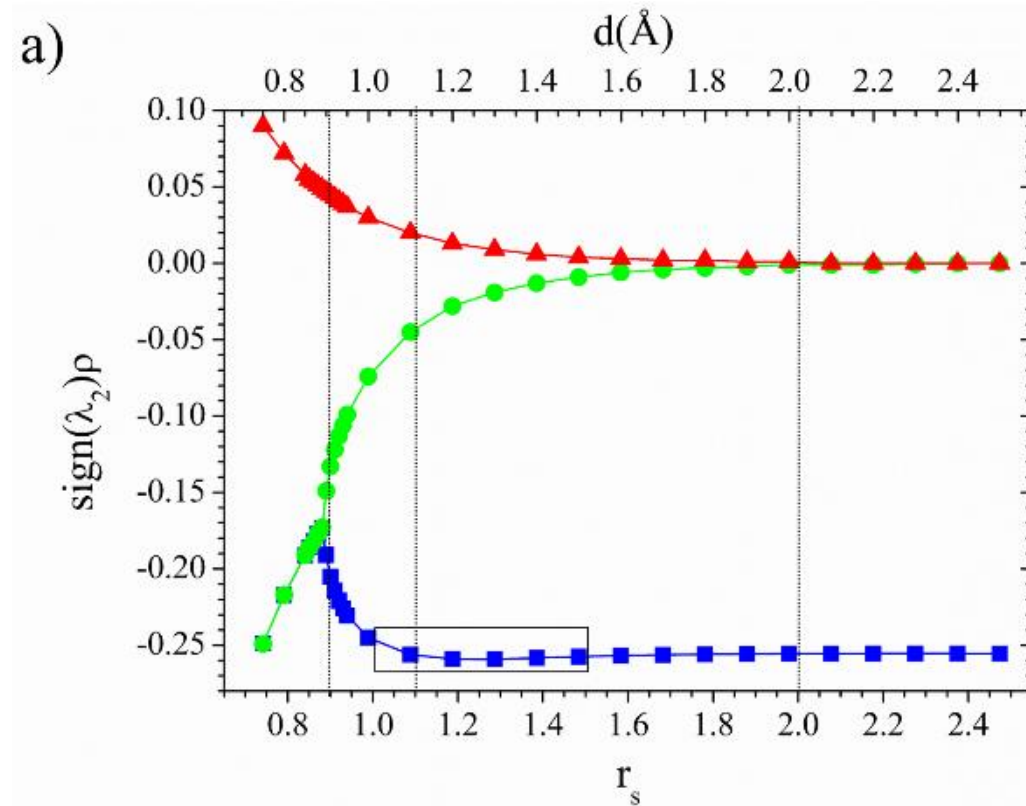
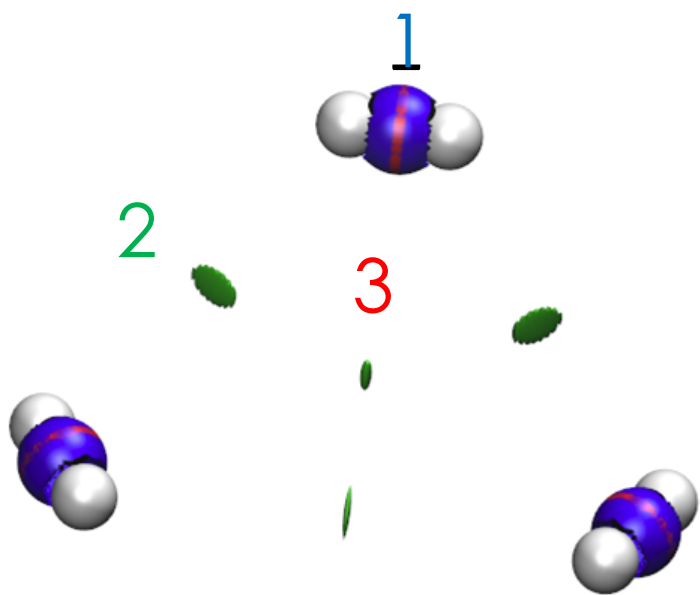
1. H-H intramolecular covalent bonds
2. Attractive intermolecular interaction (vdW)
3. Repulsive intermolecular interaction



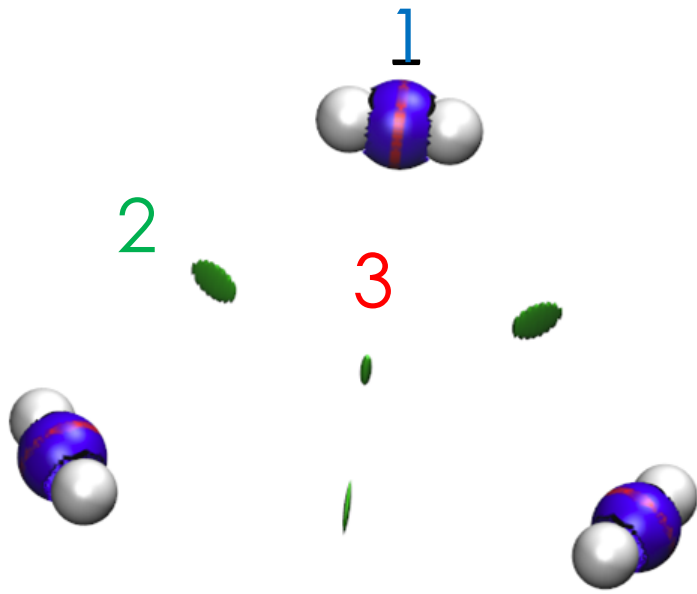
λ_2 : eigenvalue of the ρ Hessian matrix
($\lambda_1 < \lambda_2 < \lambda_3$)

$\lambda_2 < 0$: attractive interaction
 $\lambda_2 > 0$: repulsive interaction

NCI index – evolution with pressure

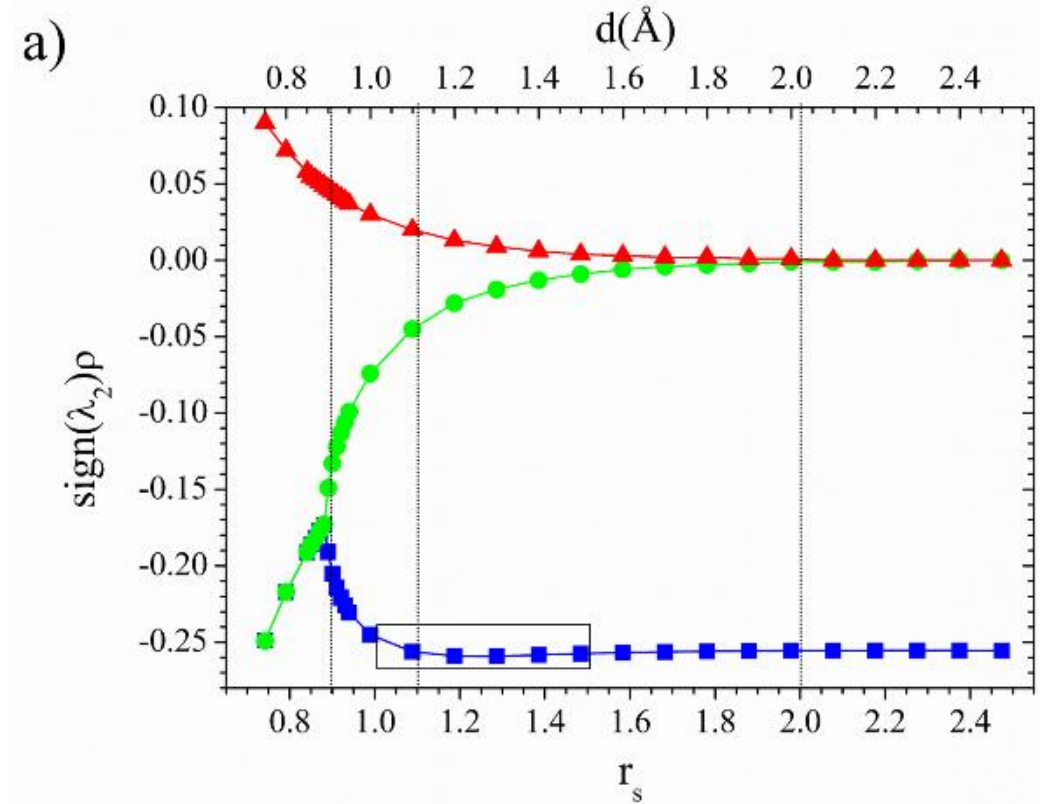


NCI index – evolution with pressure



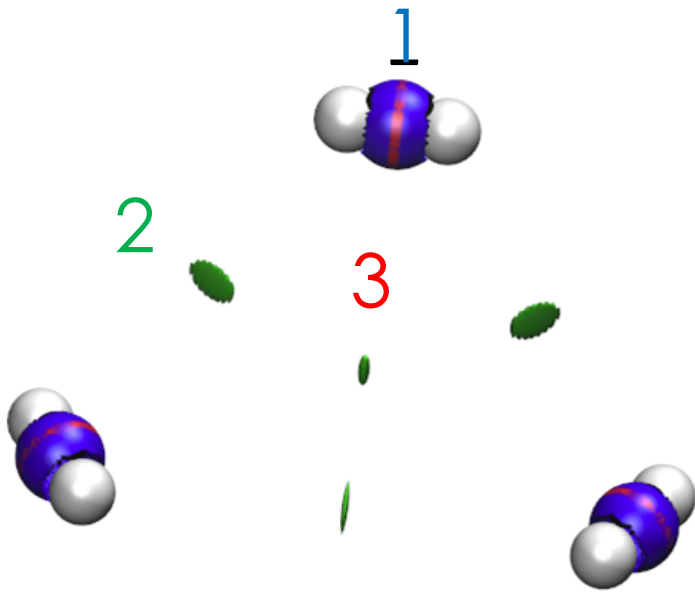
As $d \searrow$ (models $P \nearrow$)

- Intermolecular interactions strengthen (both attractive and repulsive)



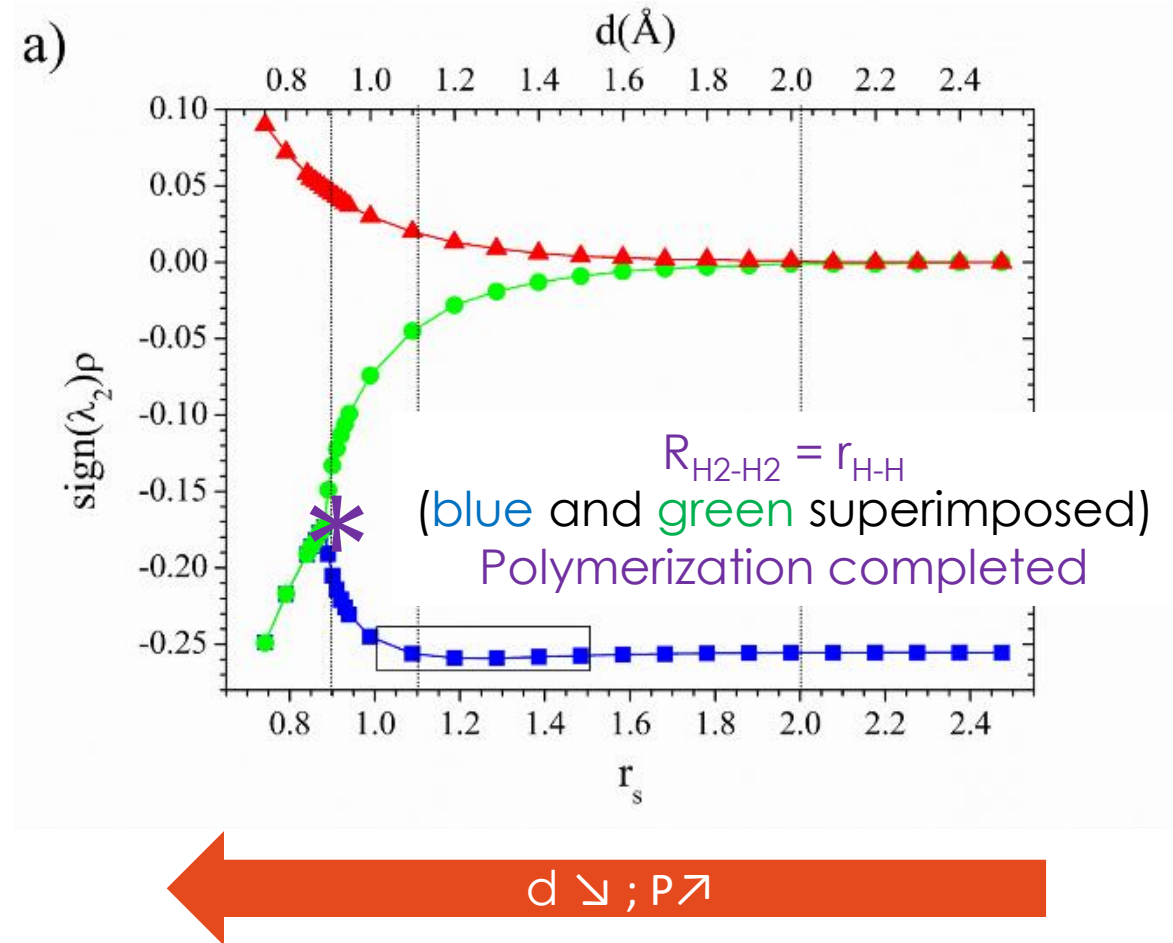
$d \searrow ; P \nearrow$

NCI index – evolution with pressure

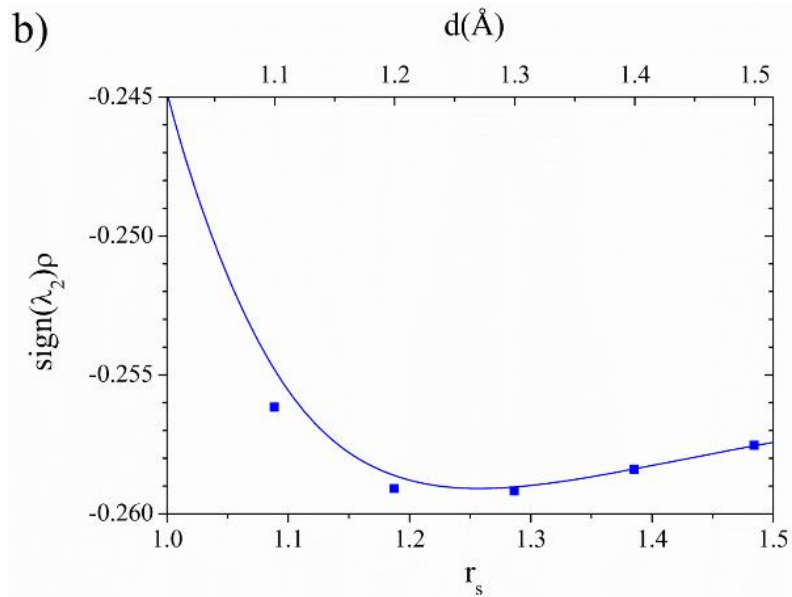


As $d \searrow$ (models $P \nearrow$)

- Intermolecular interactions strengthen (both attractive and repulsive)

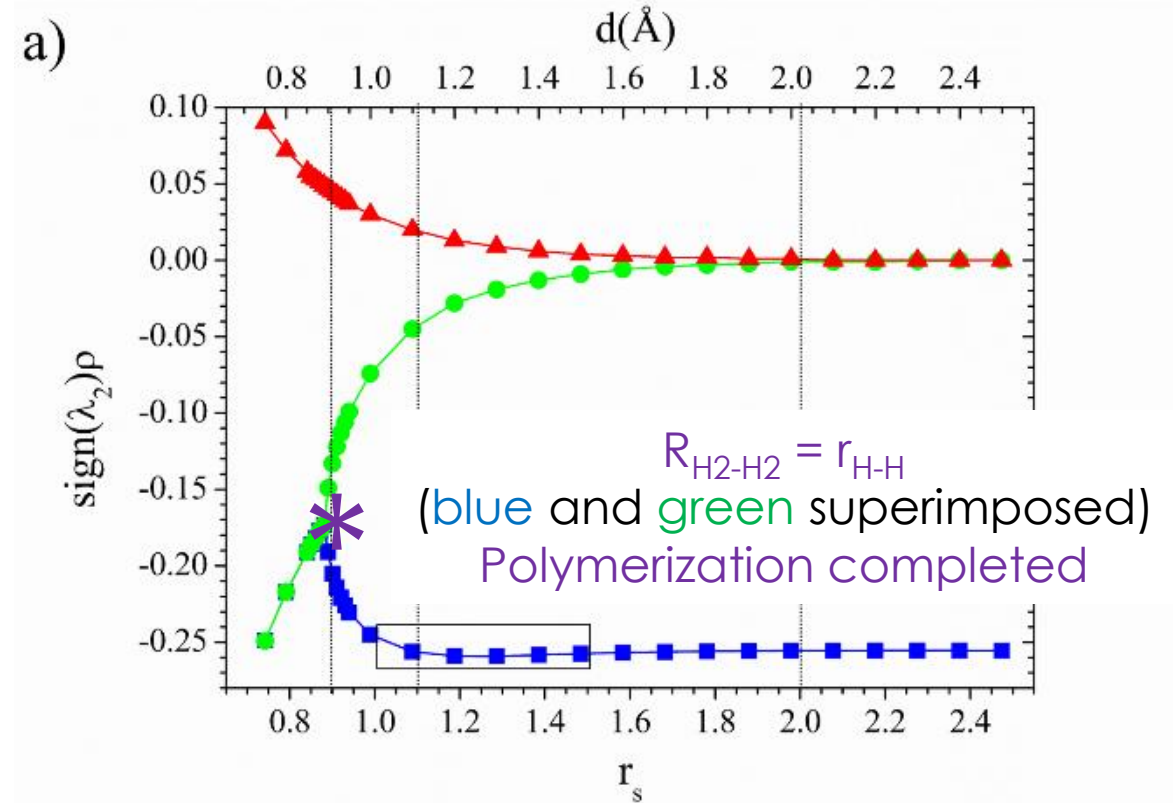


NCI index – evolution with pressure

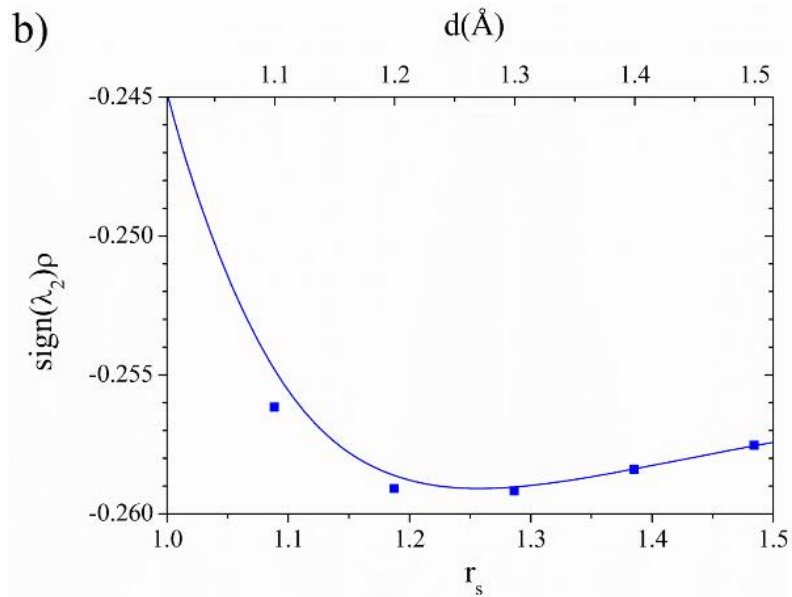


As $d \searrow$ (models P \nearrow)

- Intermolecular interactions strengthen (both attractive and repulsive)
- Intramolecular interactions
 - Strengthen ($d > 1.25$)
 - Weaken ($0.9 < d < 1.25$)
 - Strengthen again once polymerized ($d < 0.9$)

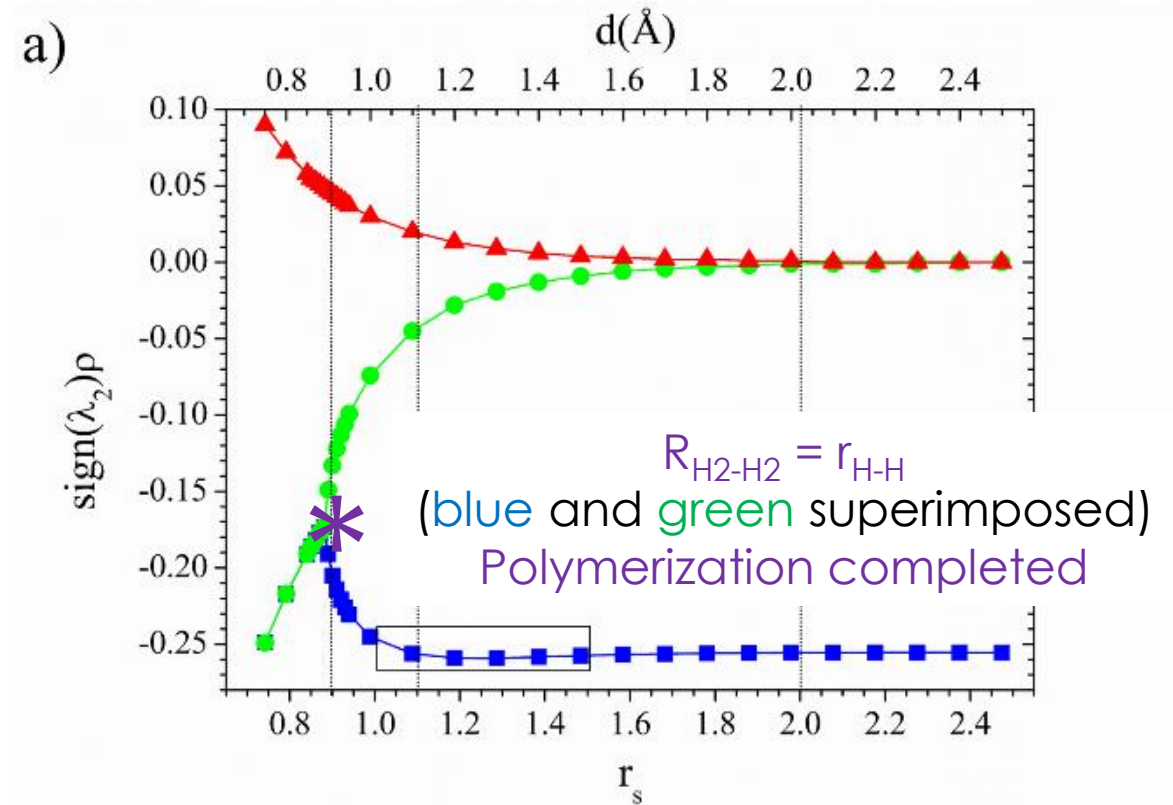


NCI index – evolution with pressure



As $d \searrow$ (models P \nearrow)

- Intermolecular interactions strengthen (both attractive and repulsive)
- Intramolecular interactions
 - Strengthen ($d > 1.25$)
 - Weaken ($0.9 < d < 1.25$)
 - Strengthen again once polymerized ($d < 0.9$)

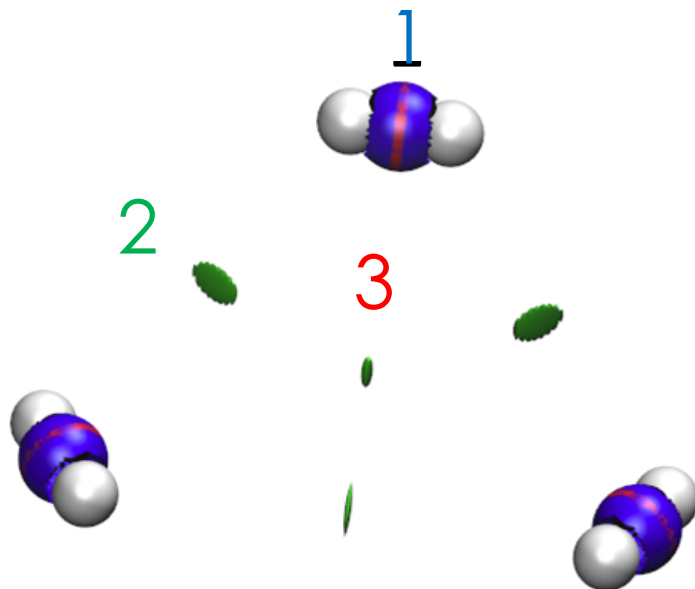


Badger's rule !

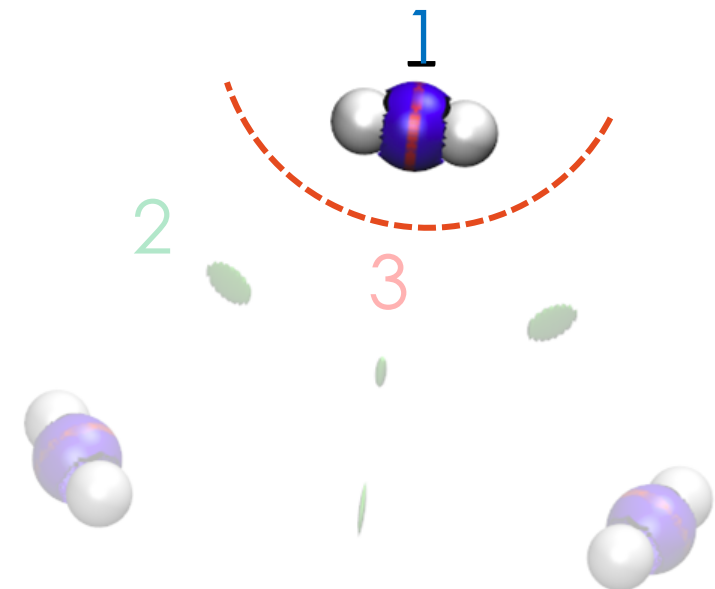
Comparison with an H₂ adapted in length

At a given d ,
comparison of the electronic distribution

H₂ of the interacting system



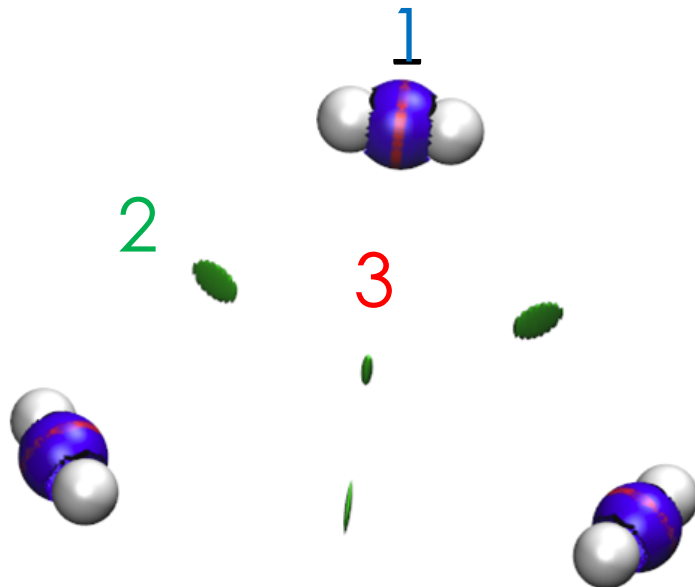
H₂ of the interacting system
Isolated from its neighbors



Comparison with an H₂ adapted in length

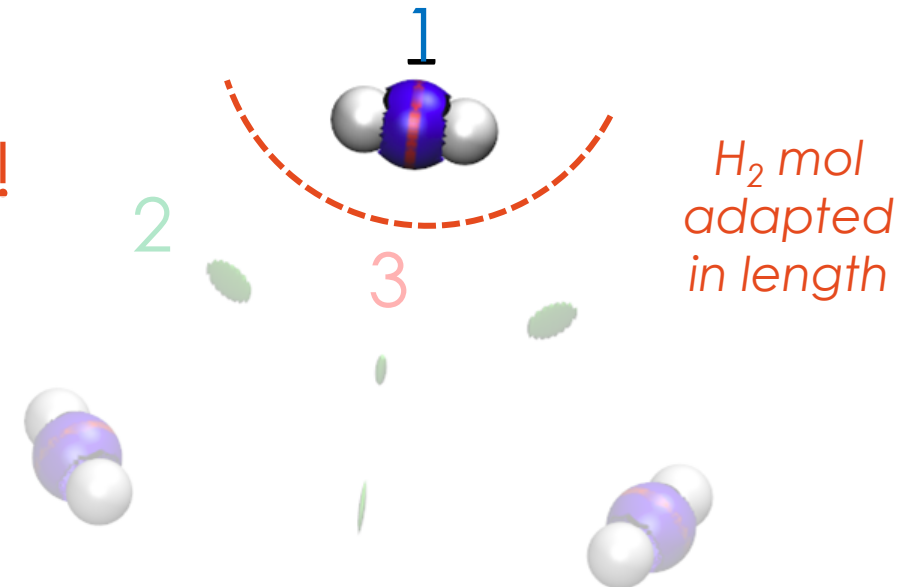
At a given d ,
comparison of the electronic distribution

H₂ of the interacting system

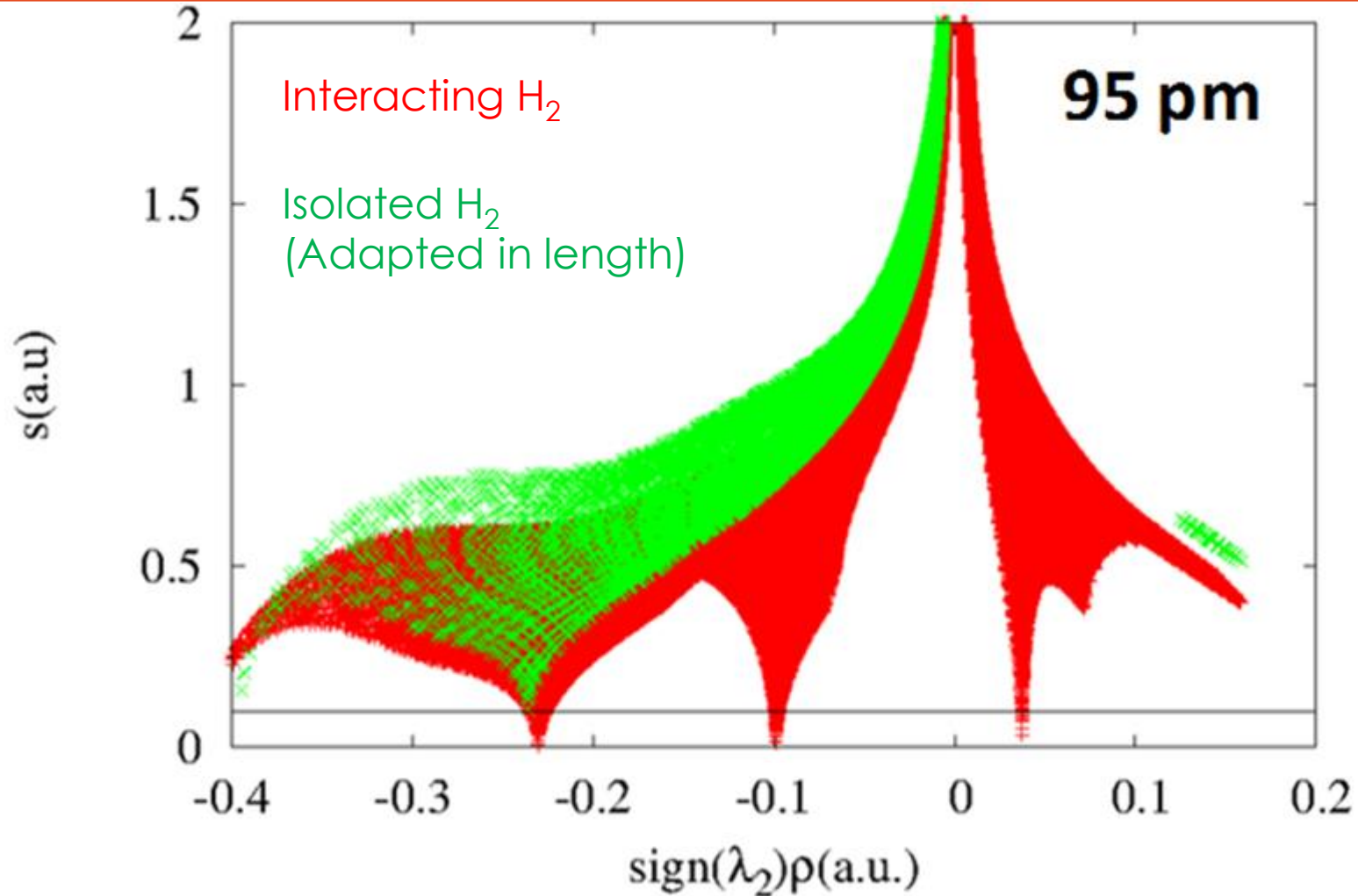
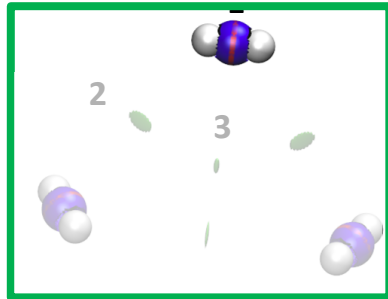
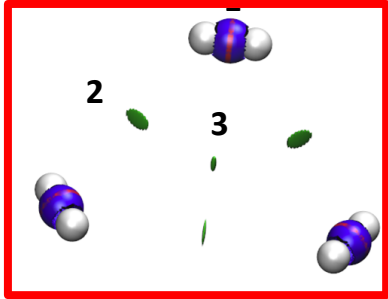


Same bond length !

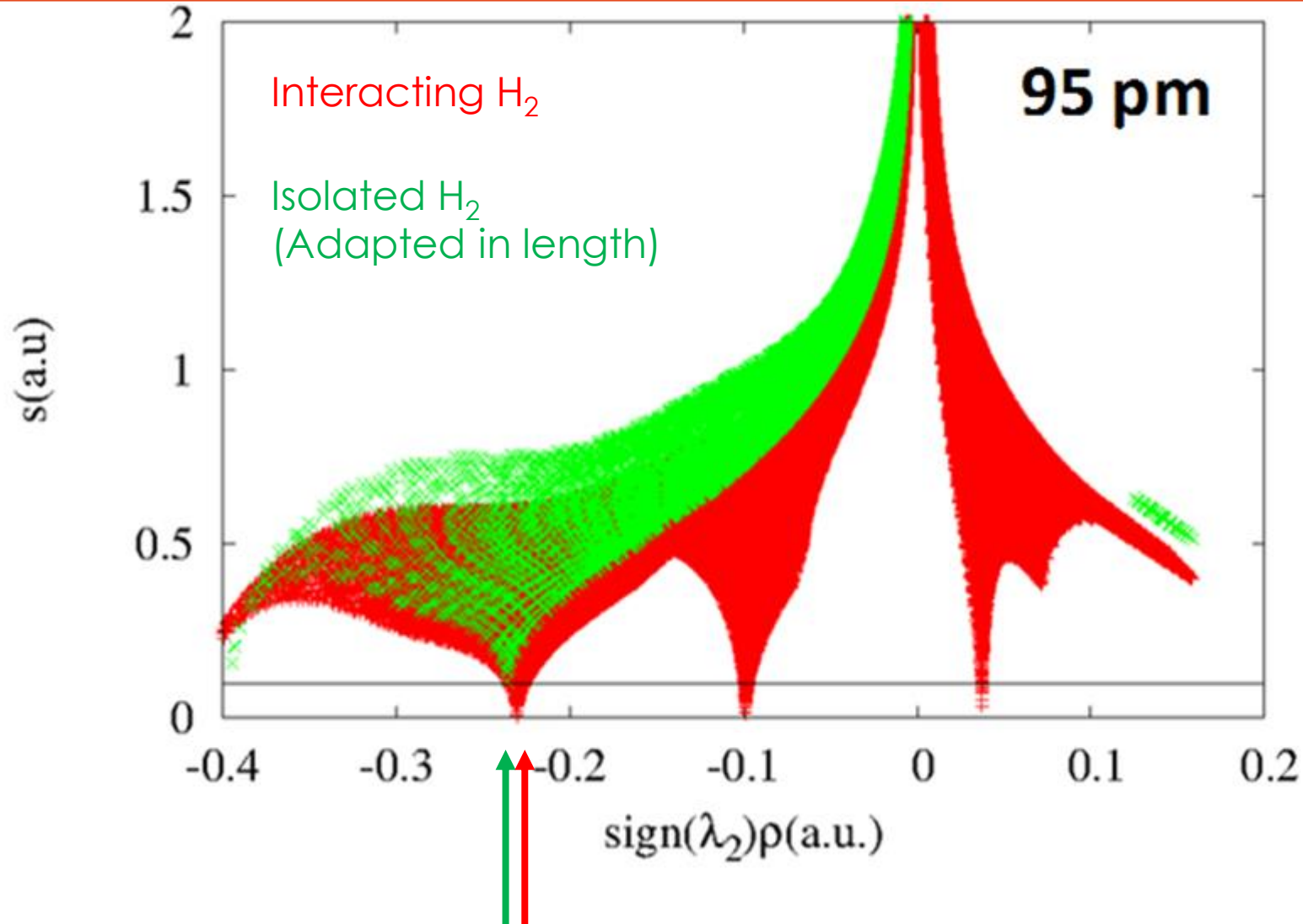
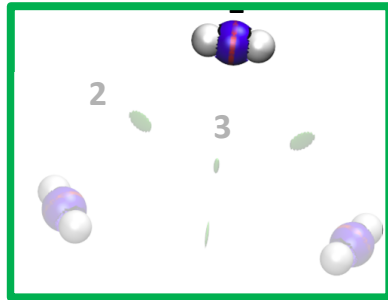
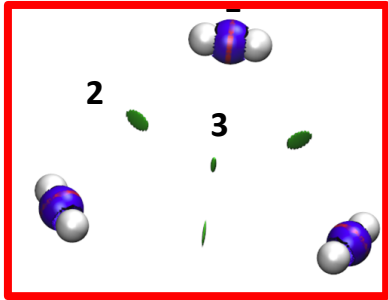
H₂ of the interacting system
Isolated from its neighbors



Comparison with an H₂ adapted in length

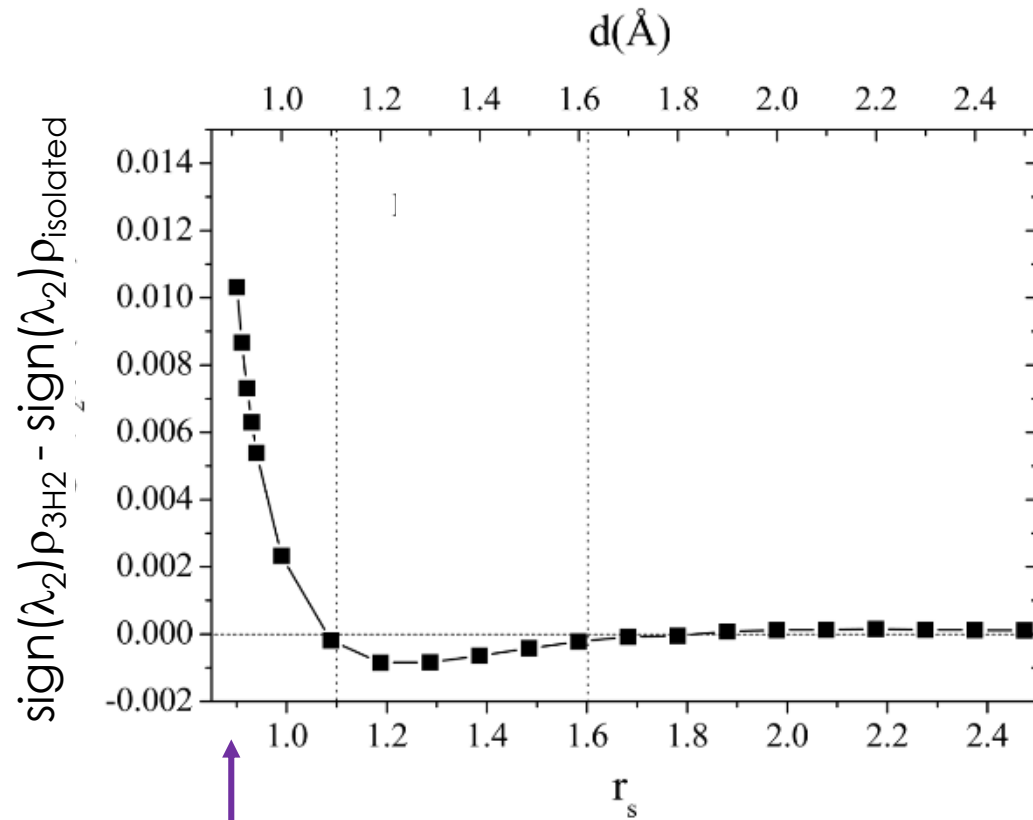


Comparison with an H₂ adapted in length



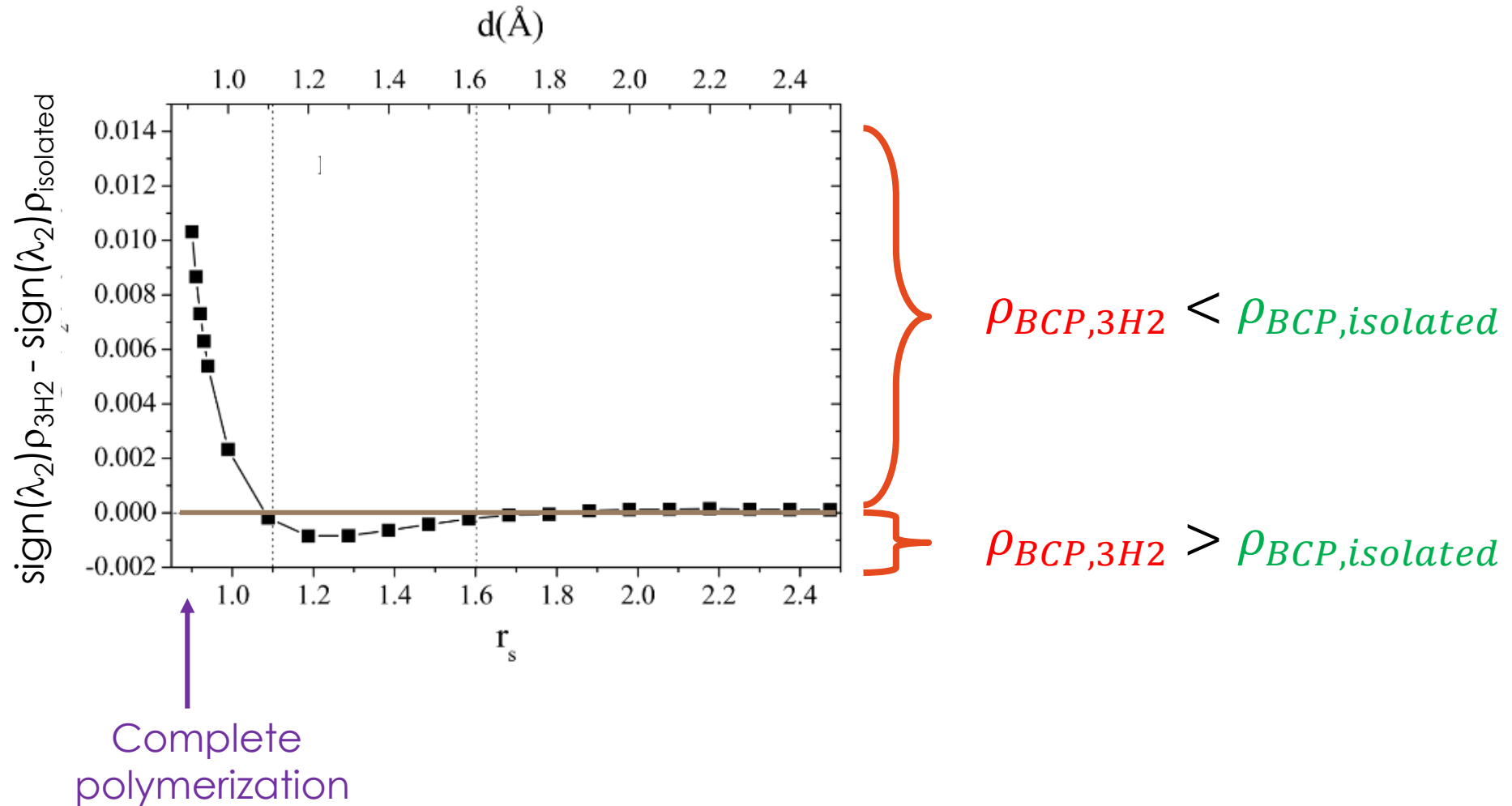
Small shift
in the density
of the
intramolecular spikes

Before complete polymerization

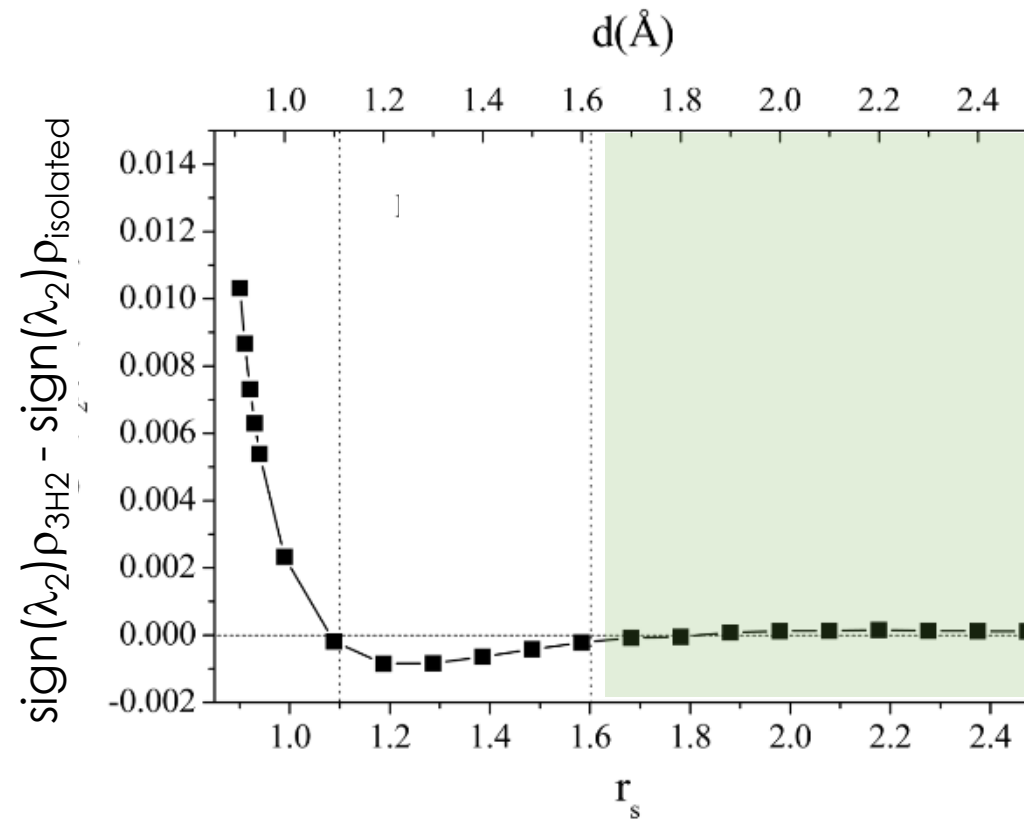


Complete
polymerization

Before complete polymerization

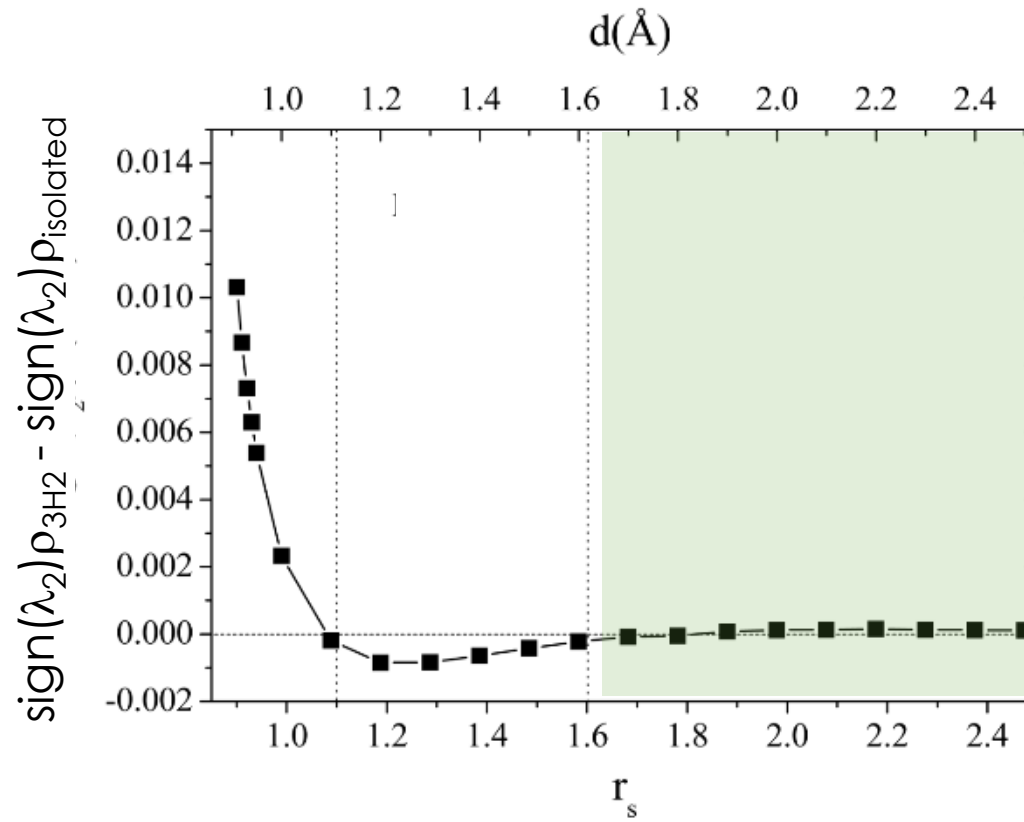


3 regimes

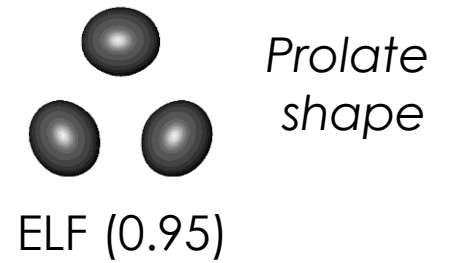


ρ organizes like
in an isolated molecule
having the same length

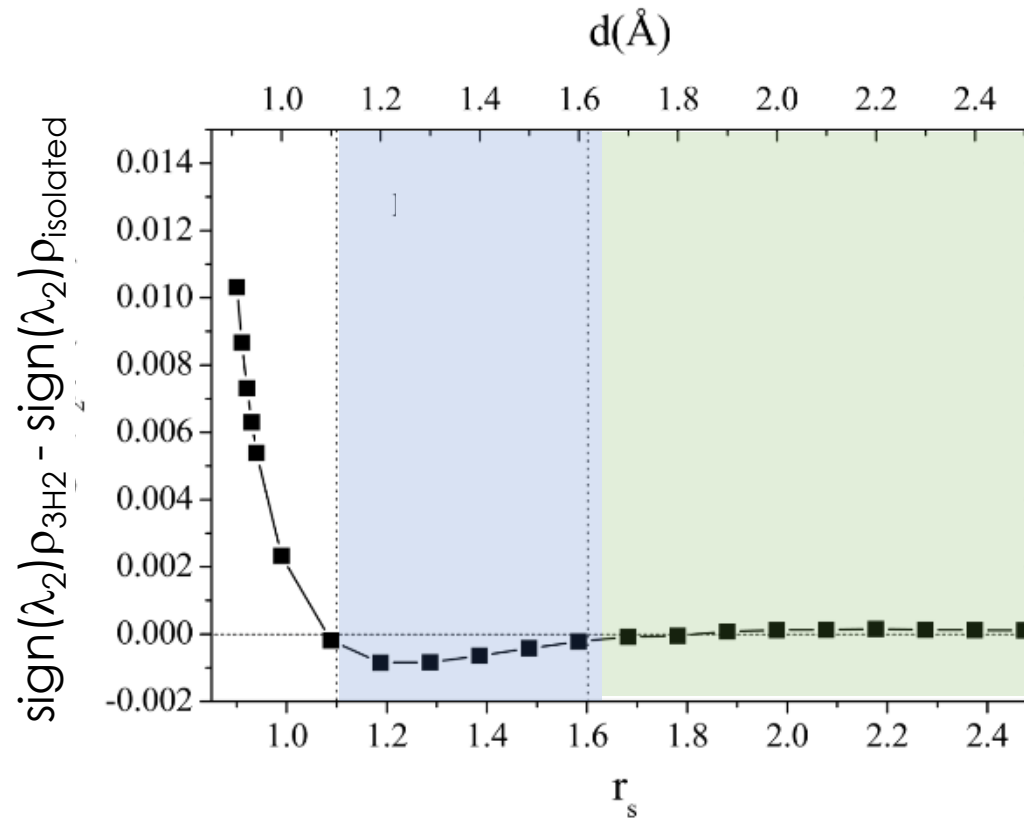
3 regimes



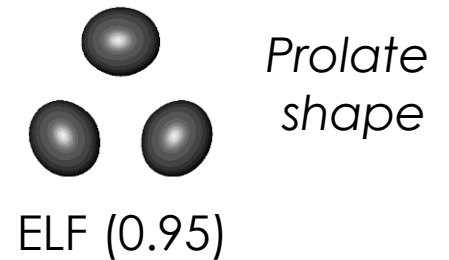
ρ organizes like
in an isolated molecule
having the same length



3 regimes



ρ organizes like
in an isolated molecule
having the same length

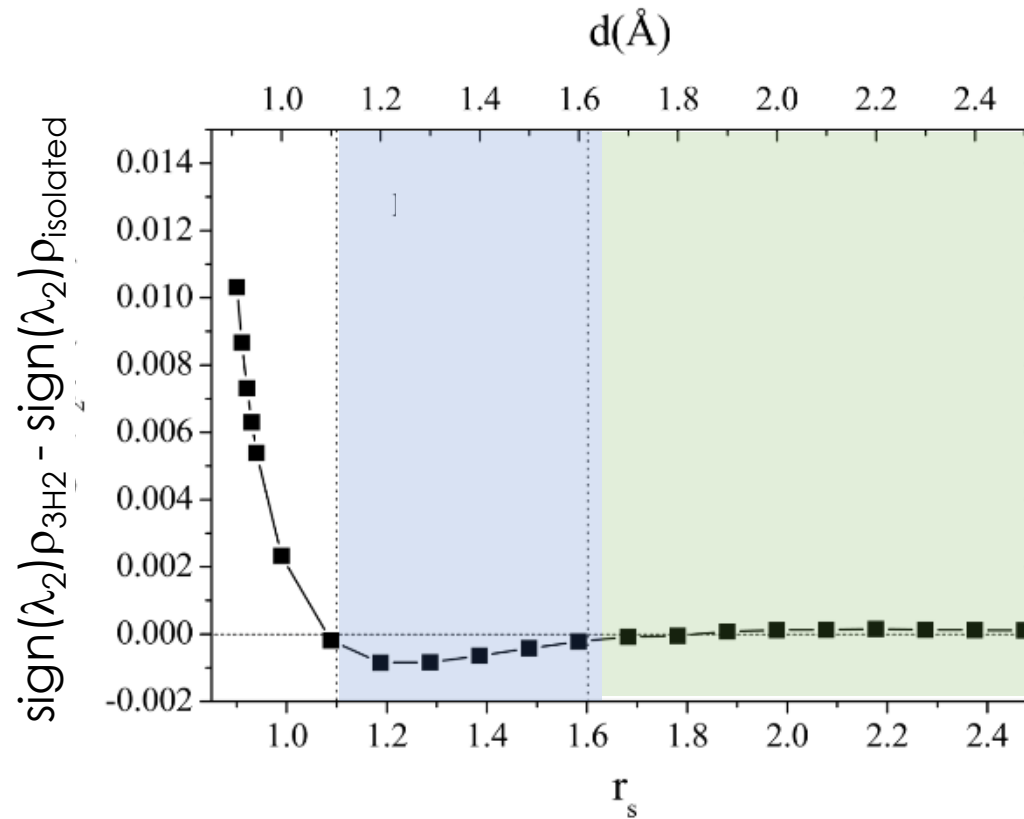


H_2 shorter than a normal mol.

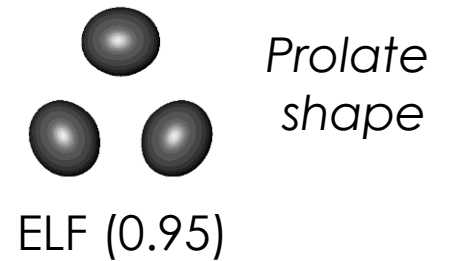
ρ_{BCP} higher than in a « shortened » H_2 mol.

ρ reorganization: inter \rightarrow intra

3 regimes



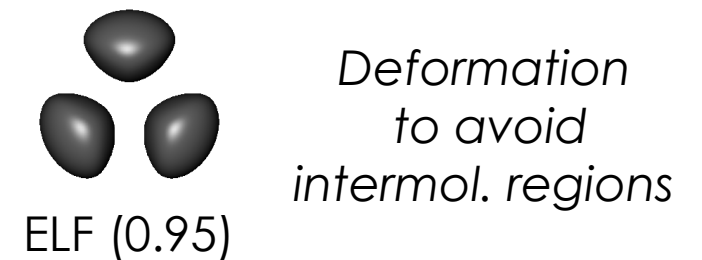
ρ organizes like
in an isolated molecule
having the same length



H_2 shorter than a normal mol.

ρ_{BCP} higher than in a « shortened » H_2 mol.

ρ reorganization: inter \rightarrow intra

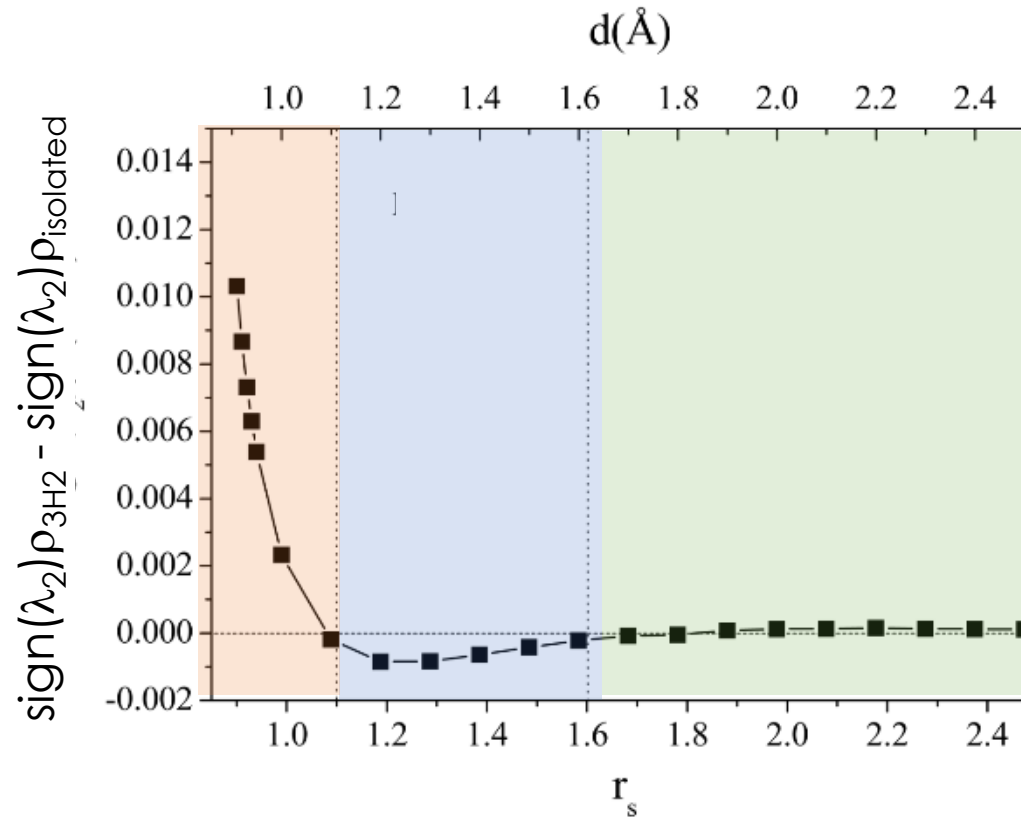


3 regimes

H₂ longer than a normal mol.

ρ_{BCP} smaller than in a « elongated » H₂ mol.

ρ reorganization: intra \rightarrow inter

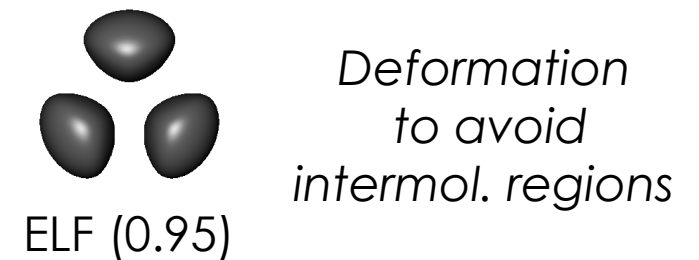
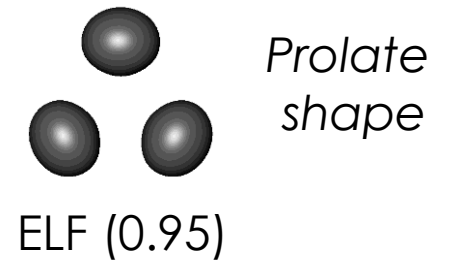


H₂ shorter than a normal mol.

ρ_{BCP} higher than in a « shortened » H₂ mol.

ρ reorganization: inter \rightarrow intra

ρ organizes like in an isolated molecule having the same length



3 regimes

H₂ longer than a normal mol.

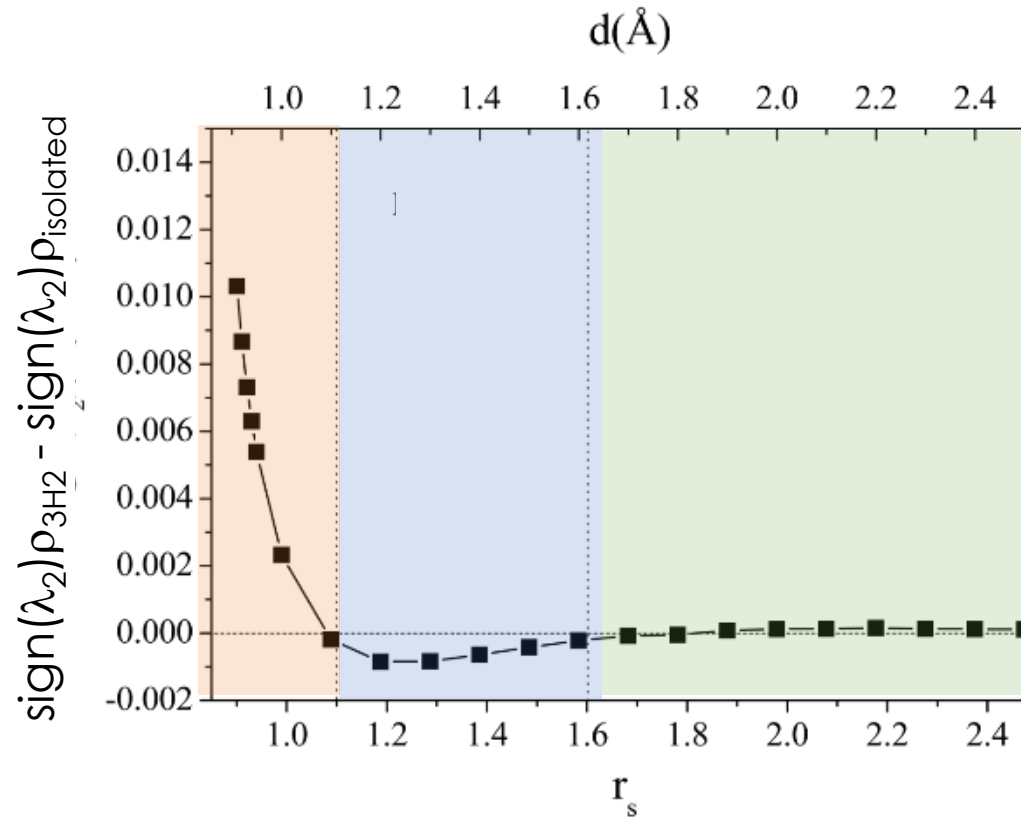
ρ_{BCP} smaller than in a « elongated » H₂ mol.

ρ reorganization: intra \rightarrow inter



ELF (0.95)

Retreat in the intramol.region.
Bonds are breaking.

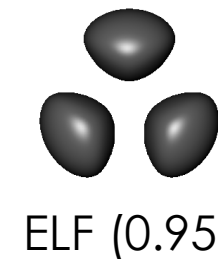
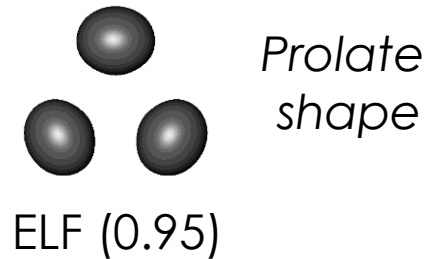


H₂ shorter than a normal mol.

ρ_{BCP} higher than in a « shortened » H₂ mol.

ρ reorganization: inter \rightarrow intra

ρ organizes like in an isolated molecule having the same length



Deformation to avoid intermol. regions

3 regimes

H_2 longer than a normal mol.

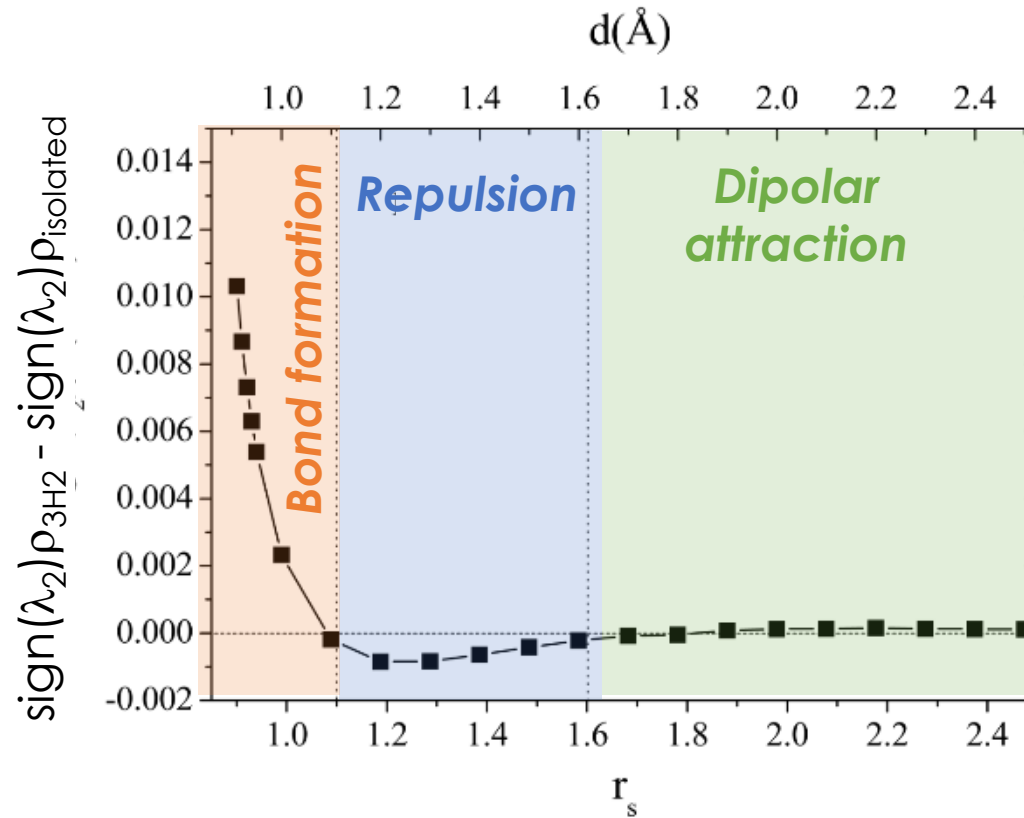
ρ_{BCP} smaller than in a « elongated » H_2 mol.

ρ reorganization: intra \rightarrow inter



ELF (0.95)

Retreat in the intramol.region. Bonds are breaking.

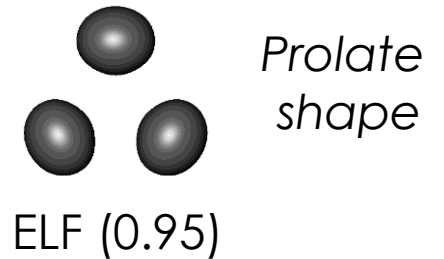


H_2 shorter than a normal mol.

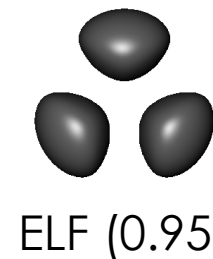
ρ_{BCP} higher than in a « shortened » H_2 mol.

ρ reorganization: inter \rightarrow intra

ρ organizes like in an isolated molecule having the same length



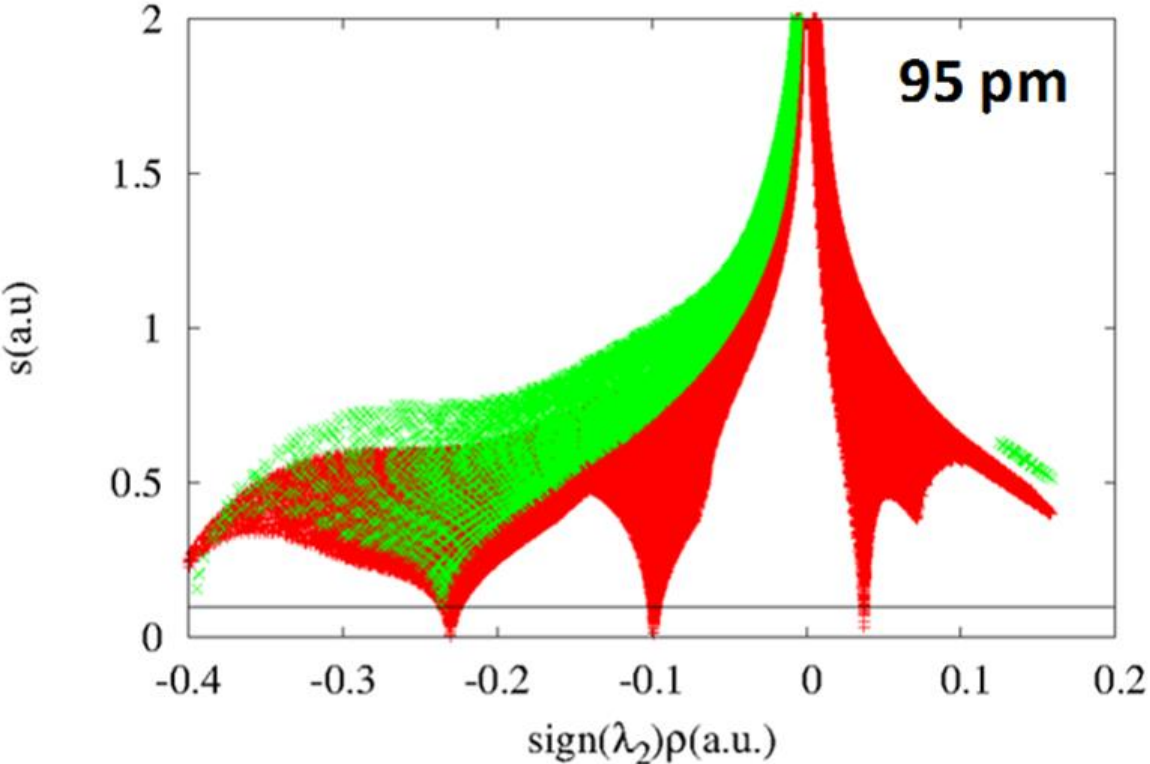
ELF (0.95)



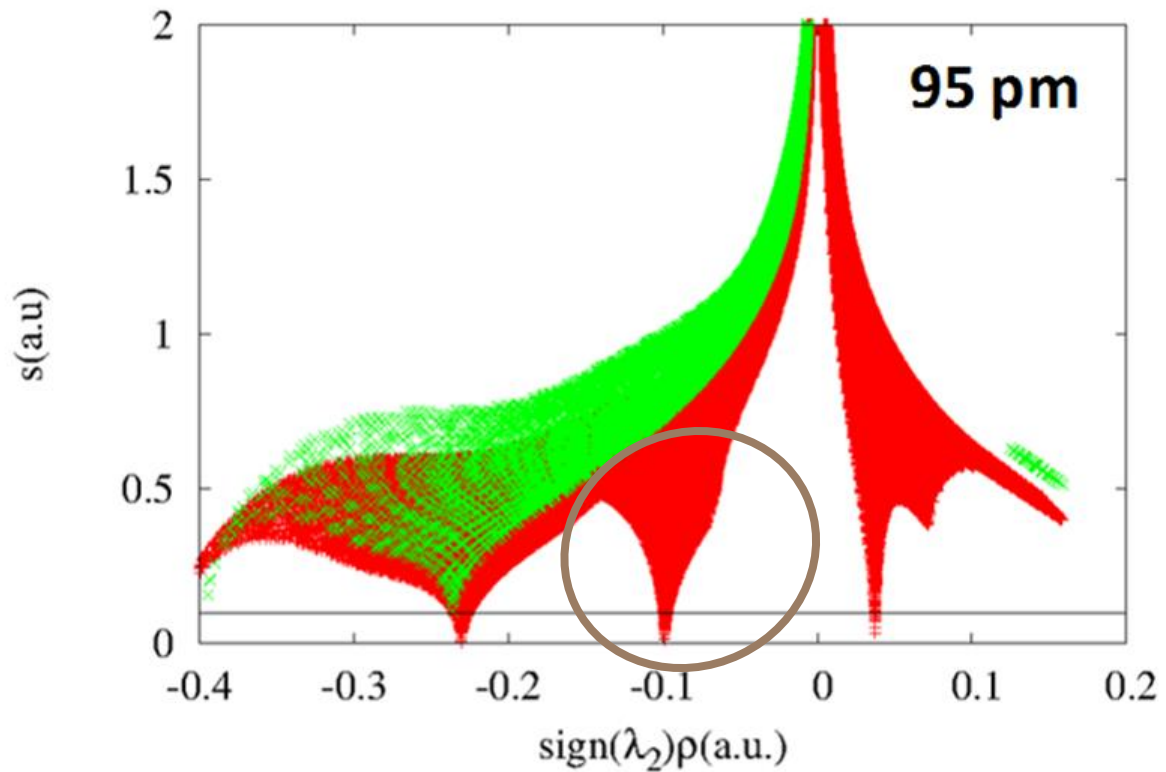
ELF (0.95)

Deformation to avoid intermol. regions

Volume of interaction

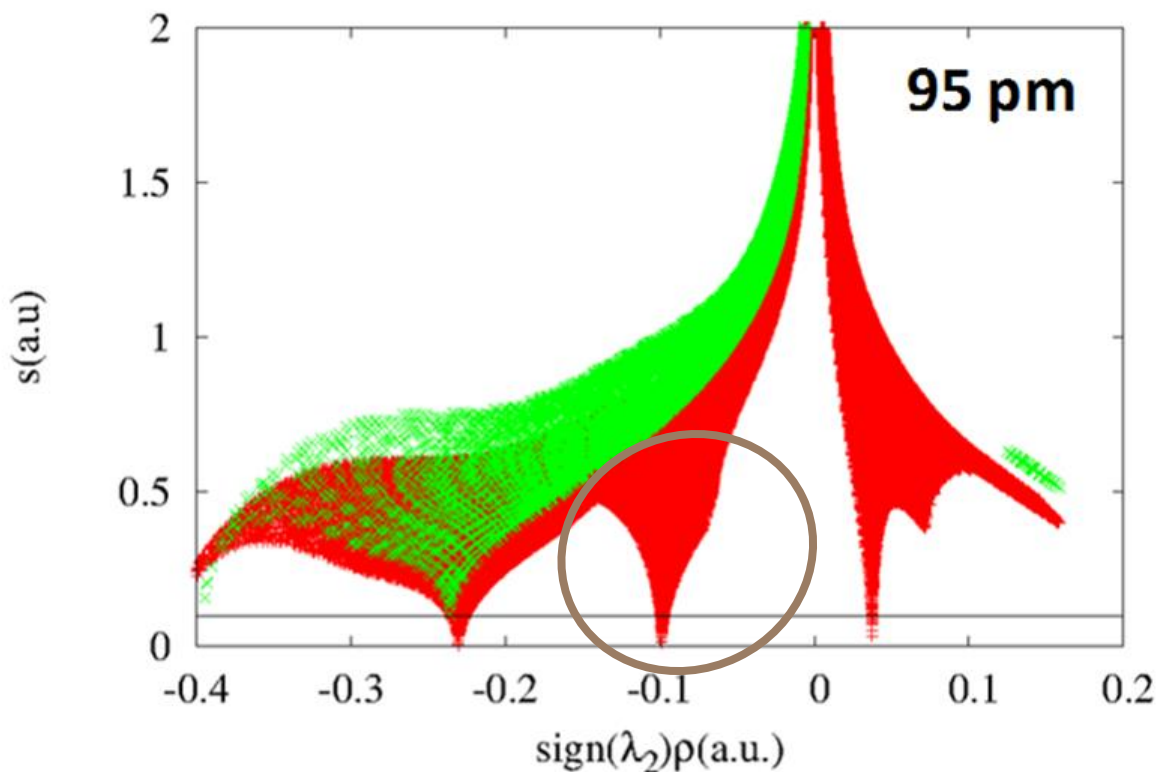


Volume of interaction

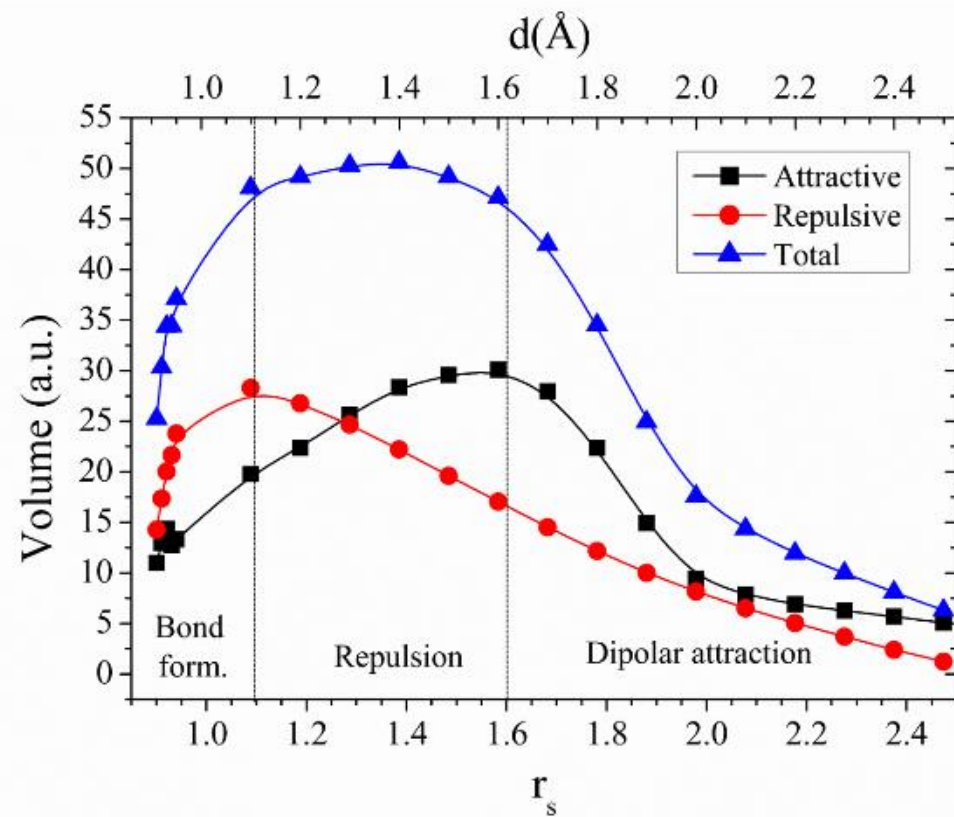


Localizing these points in the 3D space allows defining the **volume of interaction**.

Volume of interaction



Localizing these points in the 3D space allows defining the **volume of interaction**.



The global volume of interaction behaves **like in a chemical reaction** (maximum at the TS)

Analysis of H-H distances :

- Coexistence of 2 phenomena having opposite effects on the H₂ bond length
 - Physical wall (H-H bonds shorter and stiffer)
 - Orbital mixing (H-H bonds longer and weaker)

Topological tools

As H₂ molecules are coming closer and closer

- Bond length adaptation + Electronic distribution adaptation
- 3 successive regimes: dipolar attraction, repulsion, bond formation
- Relevance of a very simple non periodic model to capture the essence of the P-induced phenomenon

After squeezing hydrogen in numerical experiments ...

... experiencing squeezed time

