

Molecular structure and dynamics with DFT

the plane-wave pseudo-potential way

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Ab initio simulations

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$$i\hbar \frac{\partial \Phi(r, R; t)}{\partial t} = \left(-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial R_I^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_i^2} + V(r, R) \right) \Phi(r, R; t)$$

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The Born-Oppenheimer approximation ($M \gg m$)

$$M \ddot{R}_I = -\frac{\partial E(R)}{\partial R_I}$$

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_i^2} + V(r, R) \right) \Psi(r|R) = E(R) \Psi(r|R)$$

Density functional theory

$$V(r, R) = \frac{e^2}{2} \frac{Z_I Z_J}{|R_I - R_J|} - \frac{Z_I e^2}{|r_i - R_I|} + \frac{e^2}{2} \frac{1}{|r_i - r_j|}$$

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Kohn-Sham
Hamiltonian

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Kohn-Sham equations from functional minimization

$$E[\{\psi\}, R] = -\frac{\hbar^2}{2m} \sum_v \int \psi_v^*(r) \frac{\partial^2 \psi_v(r)}{\partial r^2} dr + \int V(r, R) \rho(r) dr + \frac{e^2}{2} \int \frac{\rho(r) \rho(r')}{|r - r'|} dr dr' + E_{xc}[\rho(r)]$$

$$E(R) = \min(E[\{\psi\}, R])$$

$$\int \psi_u^*(r) \psi_v(r) dr = \delta_{uv}$$

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Hellmann & Feynman

$$\frac{\partial E(R)}{\partial R_I} = \int \frac{\partial v(r, R)}{\partial R_I} n(r) dr$$

Solving the Kohn-Sham equations

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi_n(\mathbf{r}) = \epsilon_n \psi_n(\mathbf{r})$$

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representation &
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$$\psi_n(\mathbf{r}) \Leftrightarrow c(n, i)$$

matrix eigenvalue
problem

$$\sum_j h(i, j) c(j, n) = \epsilon_n c(i, n)$$

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- ▶ orthogonality is a plus

Bloch states & plane waves

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})$$

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$$\rho(\mathbf{r}) = \sum_{n\mathbf{k}} |\psi_{n,\mathbf{k}}(\mathbf{r})|^2$$

$$= \sum_{n\mathbf{k}} |u_{n,\mathbf{k}}(\mathbf{r})|^2$$

Using plane waves

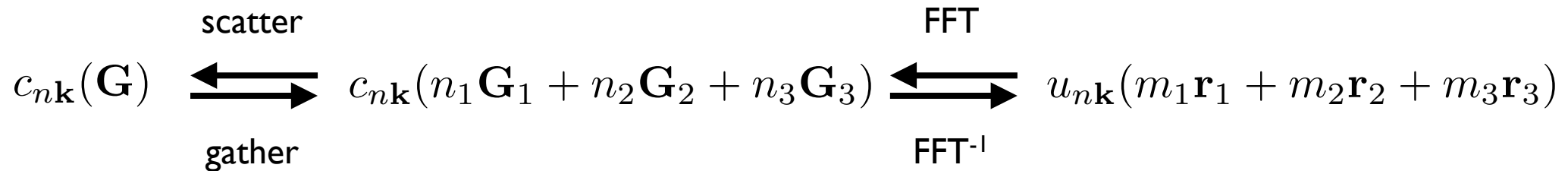
$$-\nabla^2\psi(\mathbf{r}) \quad \longmapsto \quad |\mathbf{k} + \mathbf{G}|^2 c_{n\mathbf{k}}(\mathbf{G})$$

$$V(\mathbf{r})\psi(\mathbf{r}) \quad \longmapsto \quad \int e^{-i\mathbf{G}\cdot\mathbf{r}} V(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r}$$

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$$c_{n\mathbf{k}}(\mathbf{G}) \begin{array}{c} \xleftarrow{\text{scatter}} \\ \xrightarrow{\text{gather}} \end{array} c_{n\mathbf{k}}(n_1\mathbf{G}_1 + n_2\mathbf{G}_2 + n_3\mathbf{G}_3) \begin{array}{c} \xleftarrow{\text{FFT}} \\ \xrightarrow{\text{FFT}^{-1}} \end{array} u_{n\mathbf{k}}(m_1\mathbf{r}_1 + m_2\mathbf{r}_2 + m_3\mathbf{r}_3)$$

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$$V_H(\mathbf{r}) = e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' = e^2 \sum_{\mathbf{G} \neq 0} e^{i\mathbf{G}\cdot\mathbf{r}} \frac{4\pi}{G^2} \tilde{\rho}(\mathbf{G})$$

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- ☹ uniform spatial resolution (no core states!)

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$$E(\lambda) = \min \langle \Psi | H(\lambda) | \Psi \rangle$$
$$\langle \Psi | \Psi \rangle = 1$$

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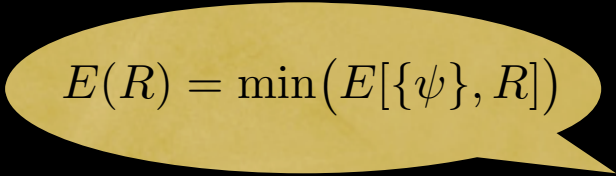
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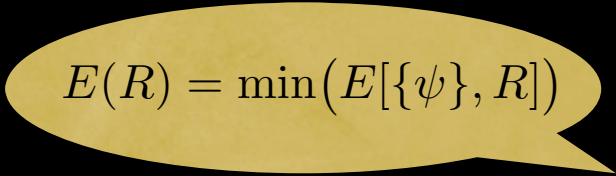

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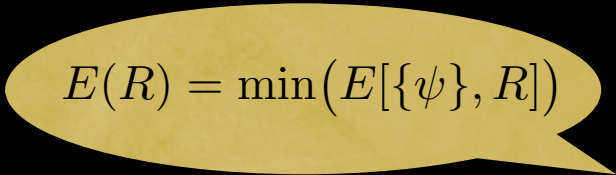

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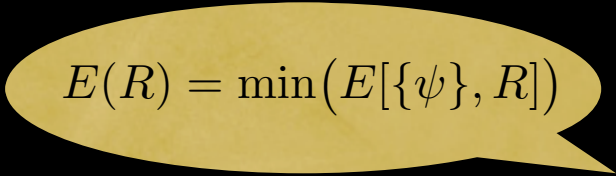
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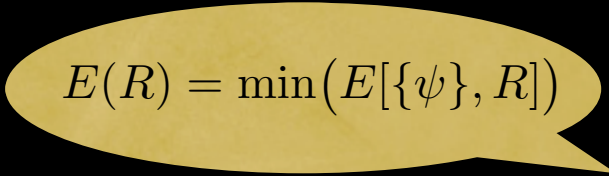
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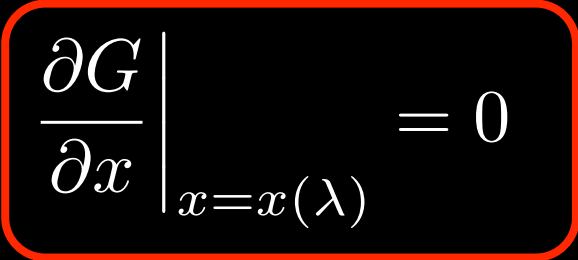
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Atomic forces

$$\mathbf{F}(\mathbf{R}) = - \overset{\text{HF}}{\int \rho(\mathbf{r}) \frac{\partial v(\mathbf{r} - \mathbf{R})}{\partial \mathbf{R}} d\mathbf{r}} - \overset{\text{Pulay}}{\int V(\mathbf{r}) \left. \frac{\partial \rho(\mathbf{r})}{\partial \mathbf{R}} \right|_P d\mathbf{r}}$$

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HF Pulay

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for PW's

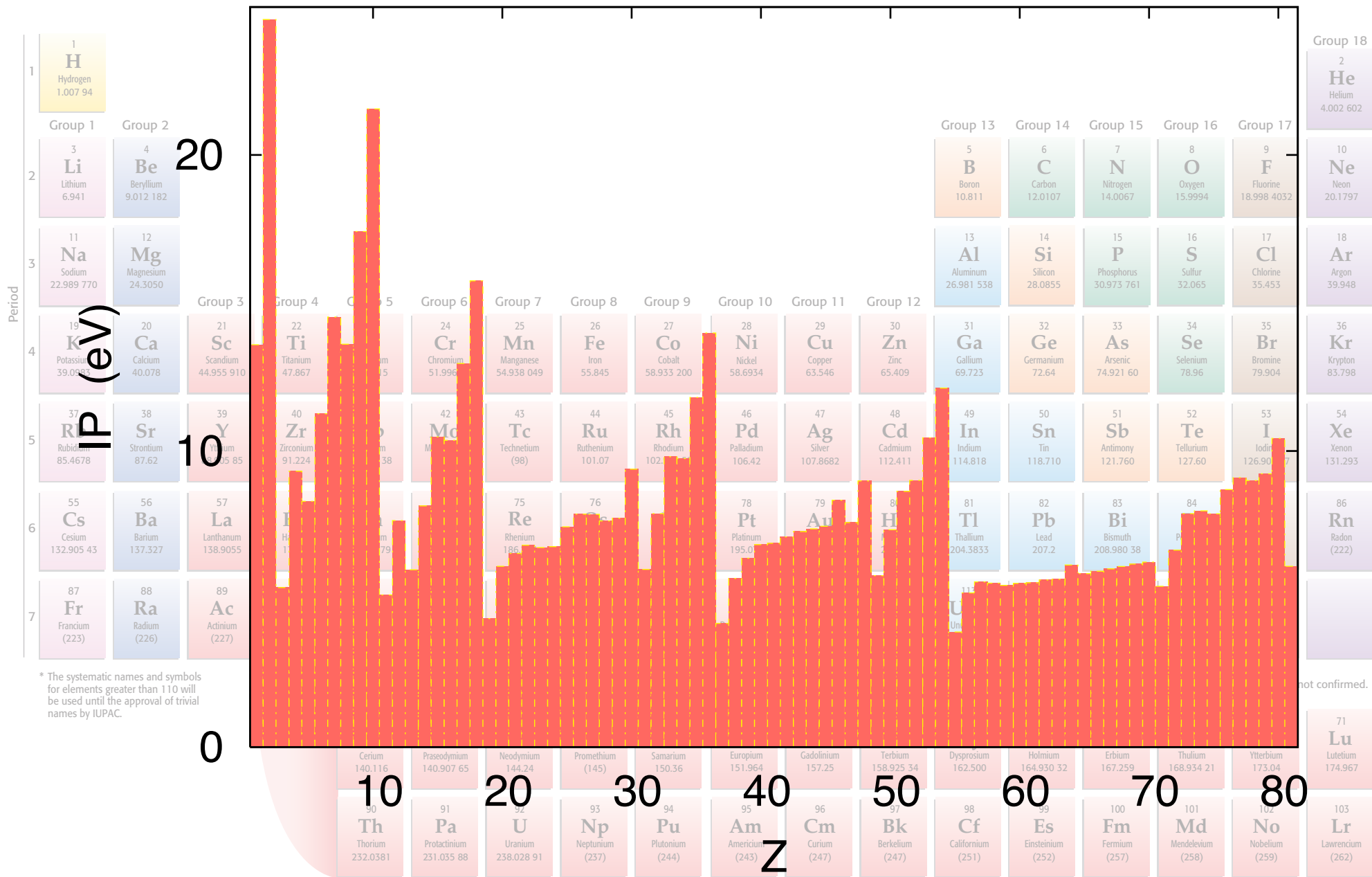
$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{R}} \Big|_P = \sum_n \sum_{ij} c(i, n) c(j, n) \left[\frac{\partial \phi_i(\mathbf{r})}{\partial \mathbf{R}} \phi_j(\mathbf{r}) + \phi_i(\mathbf{r}) \frac{\partial \phi_j(\mathbf{r})}{\partial \mathbf{R}} \right]$$

Period	1											Group 18																			
		1 H Hydrogen 1.007 94											2 He Helium 4.002 602																		
	2	Group 1	3 Li Lithium 6.941	Group 2	4 Be Beryllium 9.012 182											Group 13	5 B Boron 10.811	Group 14	6 C Carbon 12.0107	Group 15	7 N Nitrogen 14.0067	Group 16	8 O Oxygen 15.9994	Group 17	9 F Fluorine 18.998 4032	10 Ne Neon 20.1797					
	3	11 Na Sodium 22.989 770	12 Mg Magnesium 24.3050	Group 3	19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955 910	Group 4	22 Ti Titanium 47.867	Group 5	23 V Vanadium 50.9415	Group 6	24 Cr Chromium 51.9961	25 Mn Manganese 54.938 049	Group 7	26 Fe Iron 55.845	Group 8	27 Co Cobalt 58.933 200	Group 9	28 Ni Nickel 58.6934	Group 10	29 Cu Copper 63.546	Group 11	30 Zn Zinc 65.409	Group 12	13 Al Aluminum 26.981 538	14 Si Silicon 28.0855	15 P Phosphorus 30.973 761	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948
	4	37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.905 85	Group 3	40 Zr Zirconium 91.224	Group 4	41 Nb Niobium 92.906 38	Group 5	42 Mo Molybdenum 95.94	Group 6	43 Tc Technetium (98)	Group 7	44 Ru Ruthenium 101.07	Group 8	45 Rh Rhodium 102.905 50	Group 9	46 Pd Palladium 106.42	Group 10	47 Ag Silver 107.8682	Group 11	48 Cd Cadmium 112.411	Group 12	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.904 47	54 Xe Xenon 131.293		
	5	55 Cs Cesium 132.905 43	56 Ba Barium 137.327	57 La Lanthanum 138.9055	Group 3	72 Hf Hafnium 178.49	Group 4	73 Ta Tantalum 180.9479	Group 5	74 W Tungsten 183.84	Group 6	75 Re Rhenium 186.207	Group 7	76 Os Osmium 190.23	Group 8	77 Ir Iridium 192.217	Group 9	78 Pt Platinum 195.078	Group 10	79 Au Gold 196.966 55	Group 11	80 Hg Mercury 200.59	Group 12	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.980 38	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)		
	6	87 Fr Francium (223)	88 Ra Radium (226)	89 Ac Actinium (227)	Group 3	104 Rf Rutherfordium (261)	Group 4	105 Db Dubnium (262)	Group 5	106 Sg Seaborgium (266)	Group 6	107 Bh Bohrium (264)	Group 7	108 Hs Hassium (277)	Group 8	109 Mt Meitnerium (268)	Group 9	110 Ds Darmstadtium (281)	Group 10	111 Uuu* Ununium (272)	Group 11	112 Uub* Unubium (285)	Group 12	113 Uut* Ununtrium (284)	114 Uuq* Ununquadium (289)	115 Uup* Ununpentium (288)					

* The systematic names and symbols for elements greater than 110 will be used until the approval of trivial names by IUPAC.

A team at Lawrence Berkeley National Laboratories reported the discovery of elements 116 and 118 in June 1999. The same team retracted the discovery in July 2001. The discovery of elements 113, 114, and 115 has been reported but not confirmed.

58 Ce Cerium 140.116	59 Pr Praseodymium 140.907 65	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925 34	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930 32	68 Er Erbium 167.259	69 Tm Thulium 168.934 21	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
90 Th Thorium 232.0381	91 Pa Protactinium 231.035 88	92 U Uranium 238.028 91	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 (262)



$$\epsilon_{1s} \sim Z^2$$

$$a_{1s} \sim \frac{1}{Z}$$

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$$I_P \sim 1$$

$$a \sim 1$$

First principle of computational physics

First principle of computational physics

If two systems have similar physical and chemical properties, their simulation should require a similar amount of computer resources

Power to the *imagination*

Power to the *imagination*

Chemically similar atoms have potentials with very different, possibly nasty, mathematical properties?

Well ...

Power to the *imagination*

Chemically similar atoms have potentials with very different, possibly nasty, mathematical properties?
Well ...

Imagine *pseudo* atoms whose chemical properties are very similar to those of *real* atoms, but whose (*pseudo*) potentials are as gentle as possible.

Properties of pseudopotentials

Properties of pseudopotentials

V_{ps} does not have core states: valence states of any given angular symmetry are the lowest-lying states of that symmetry:

ϕ_{val}^{ps} is nodeless and smooth

Properties of pseudopotentials

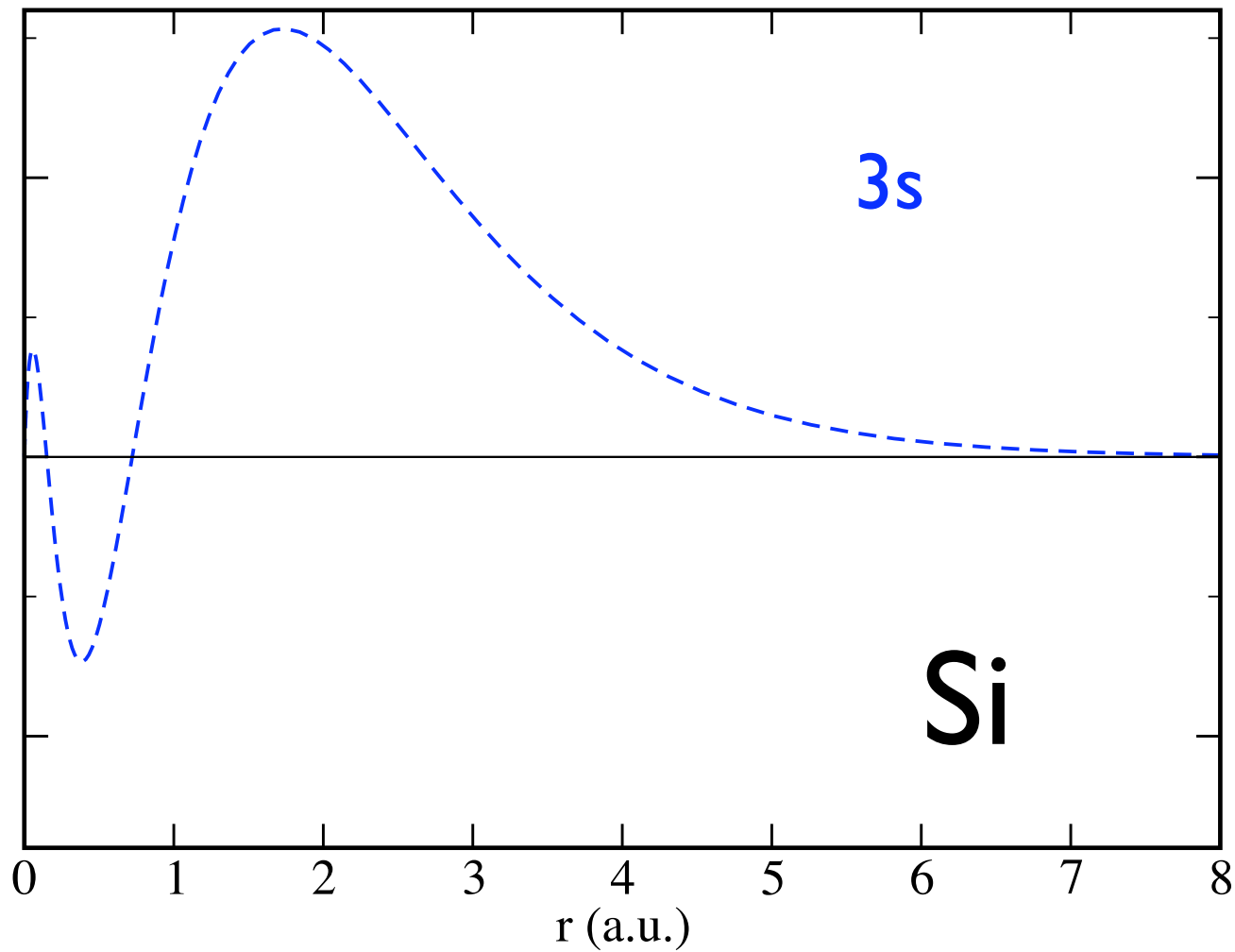
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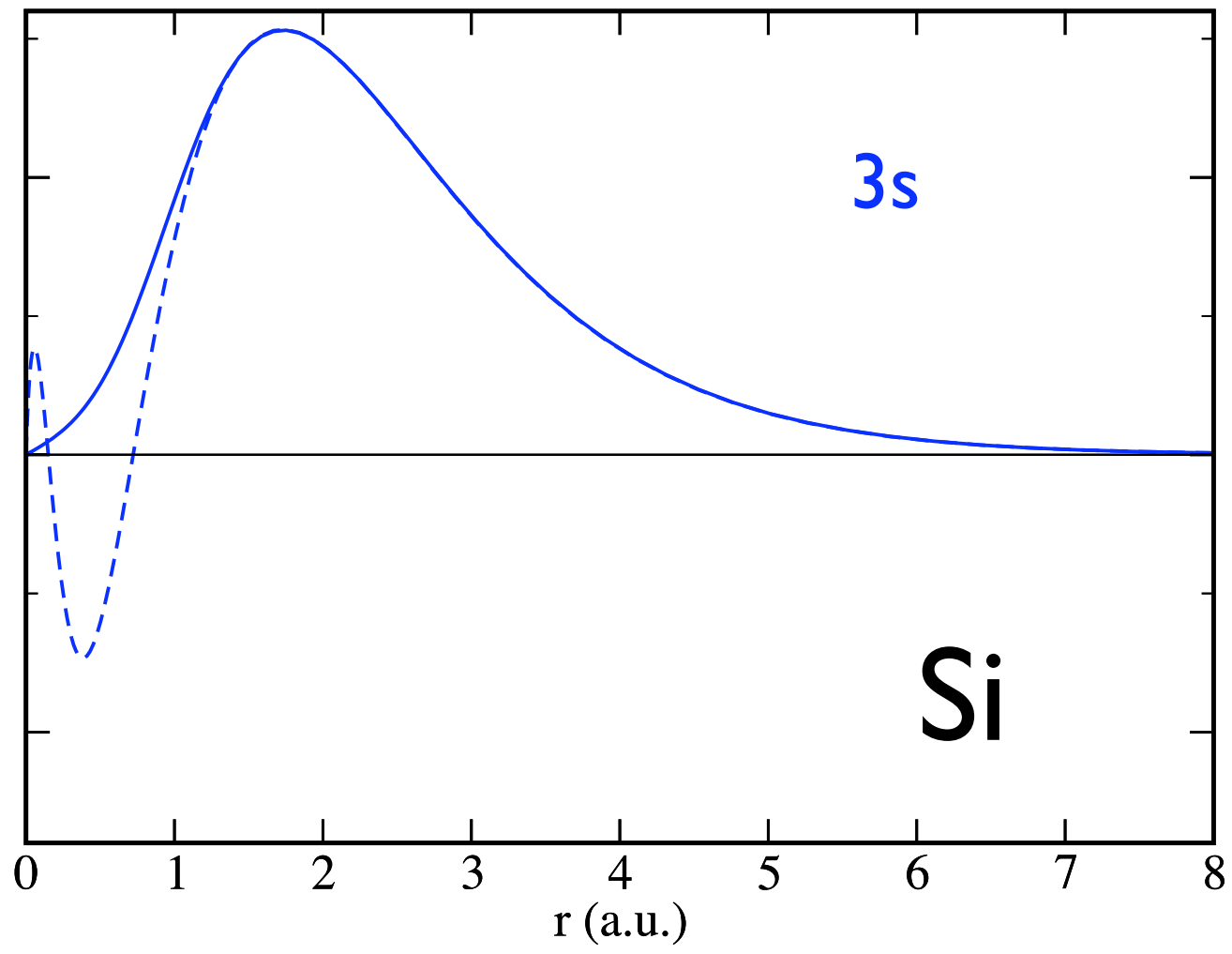
ϕ_{val}^{ps} is nodeless and smooth

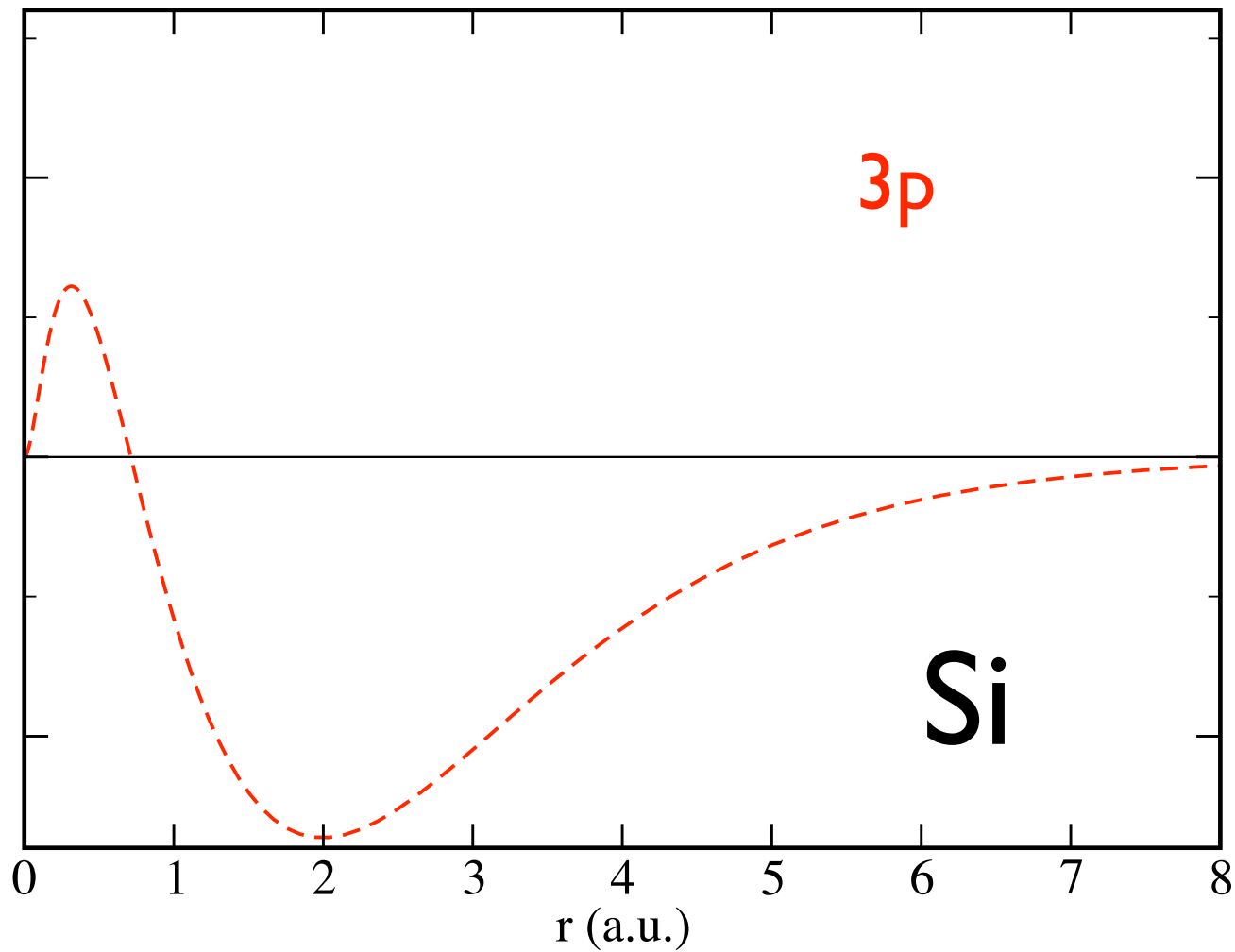
The chemical properties of the pseudo-atom are the same as those of the true atom:

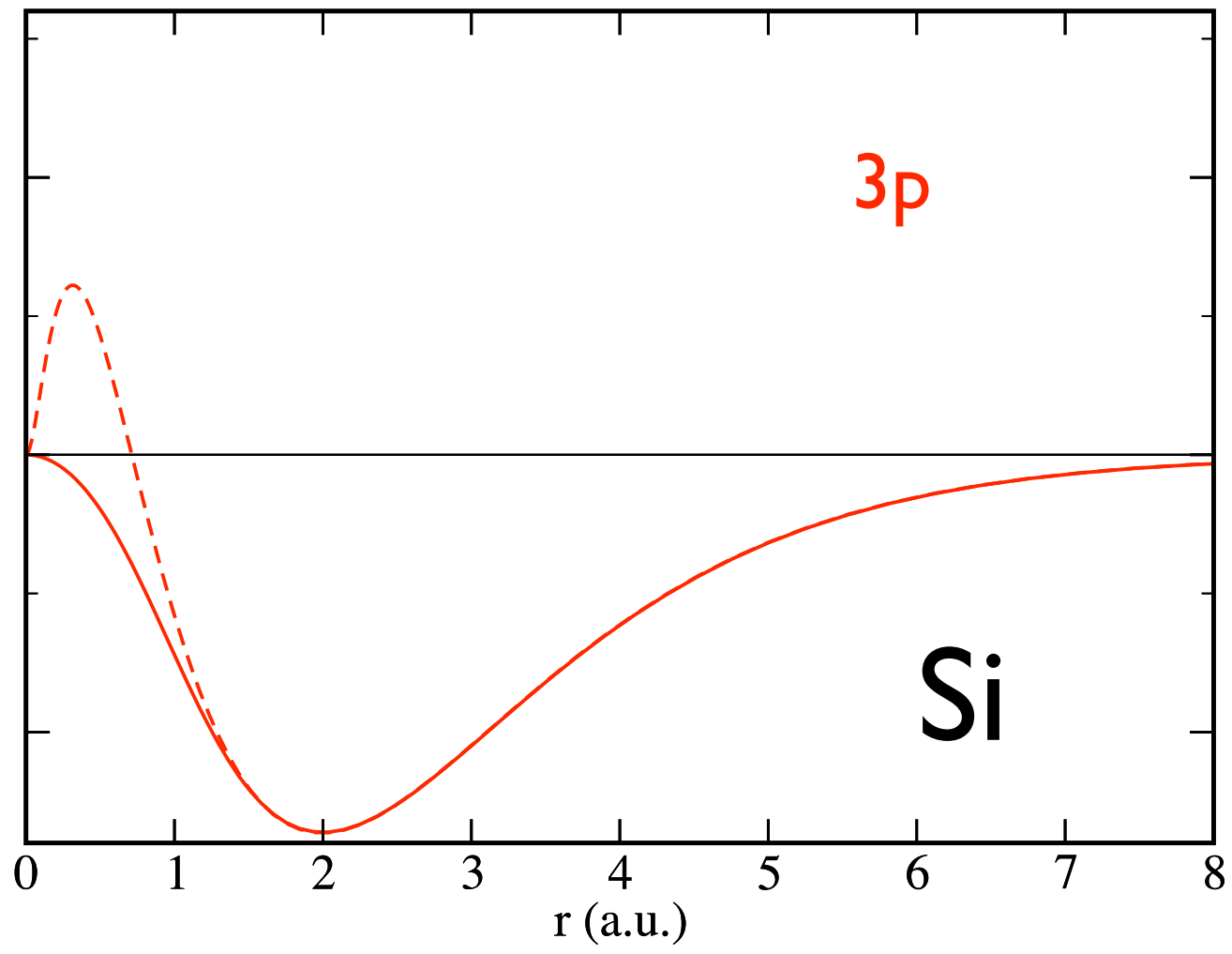
$$\epsilon_{val}^{ps} = \epsilon_{val}^{ae}$$

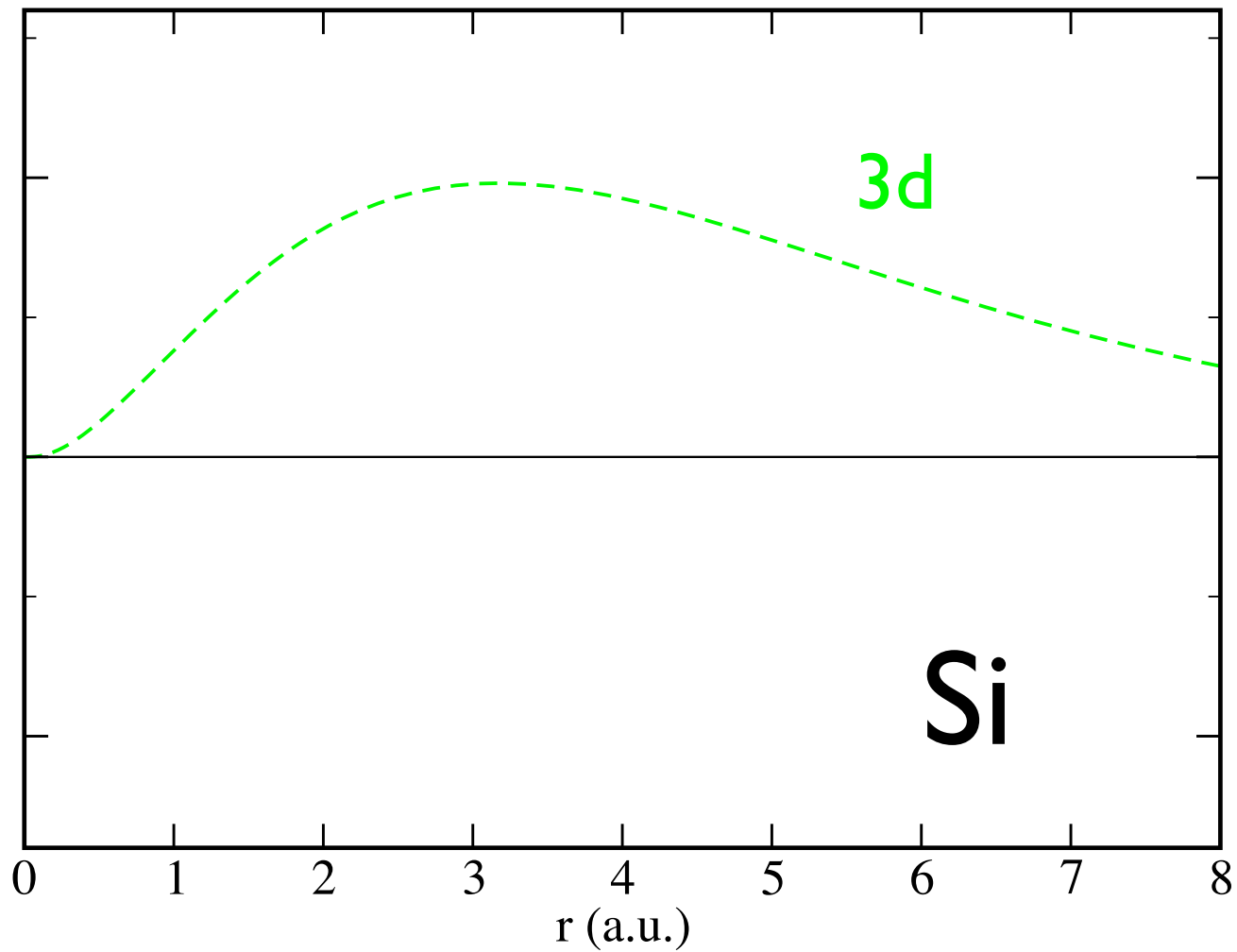
$$\phi_{val}^{ps}(r) = \phi_{val}^{ae}(r) \quad \text{for } r > r_c$$

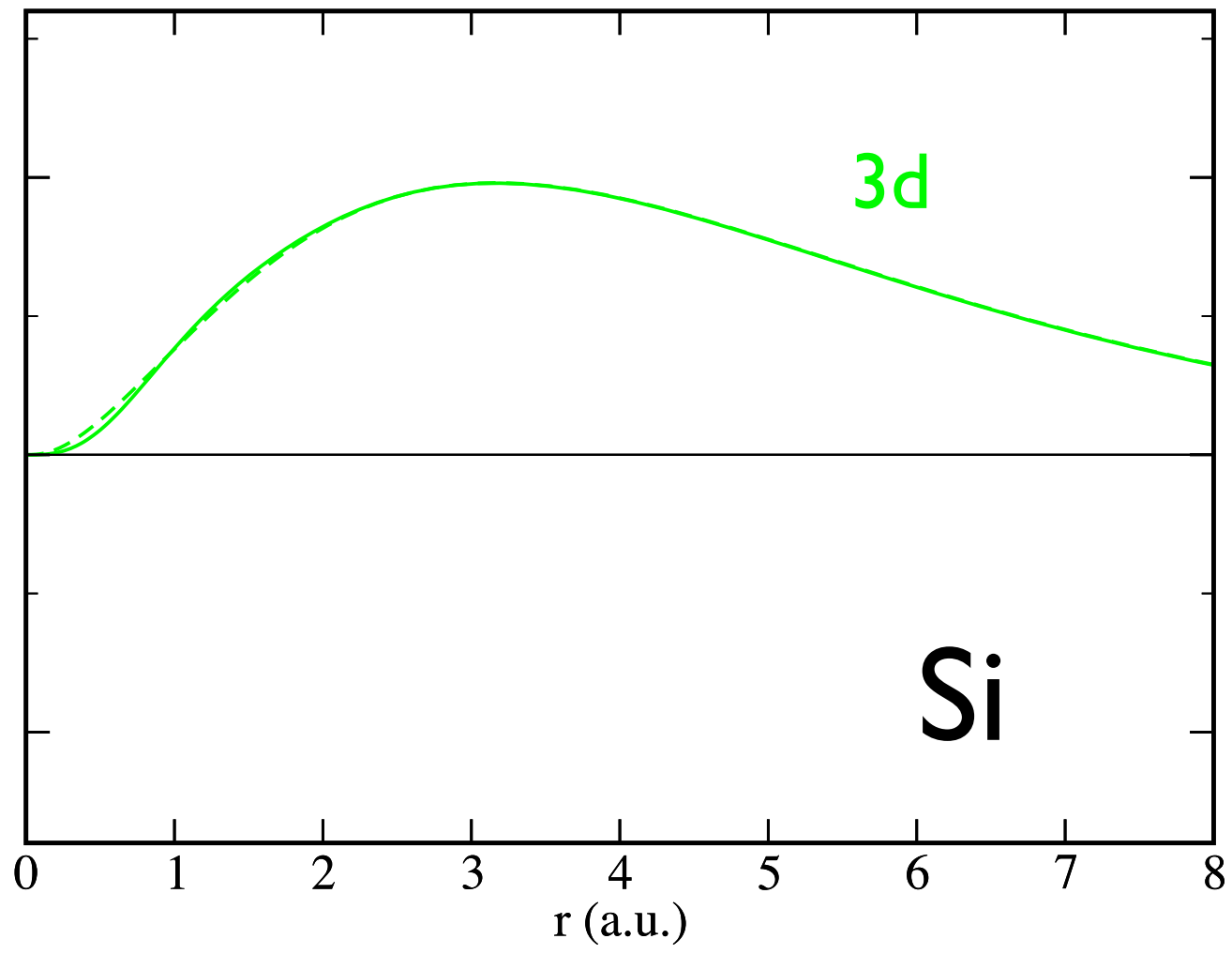




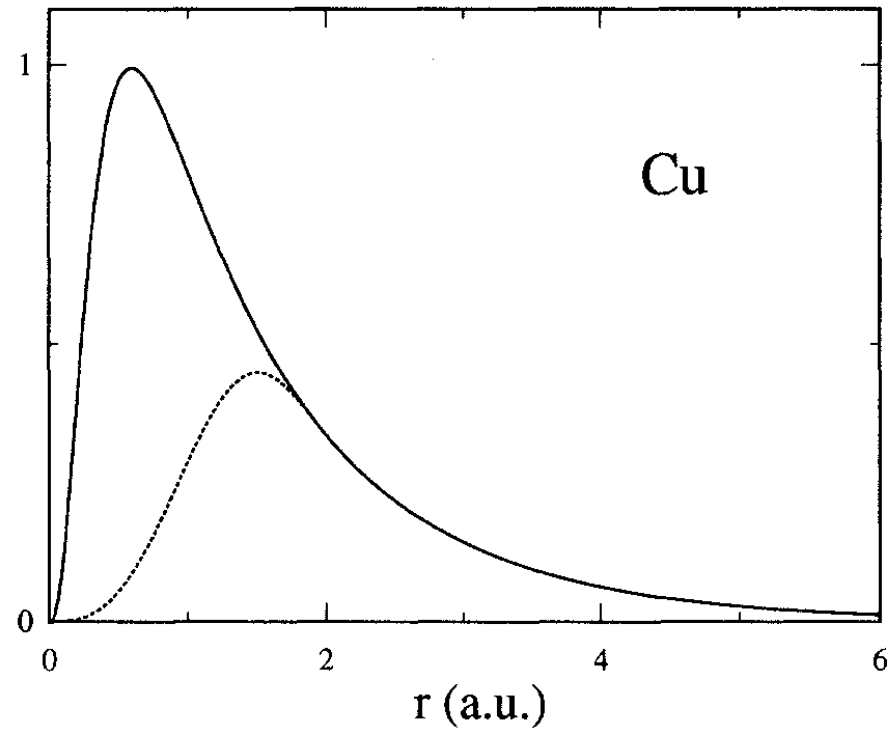




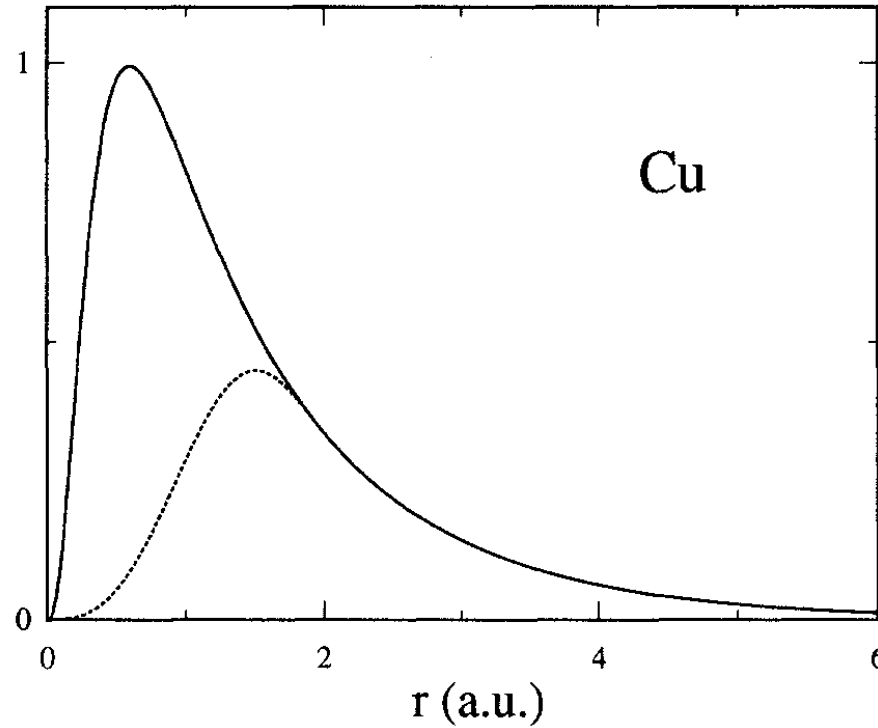




US pseudopotentials

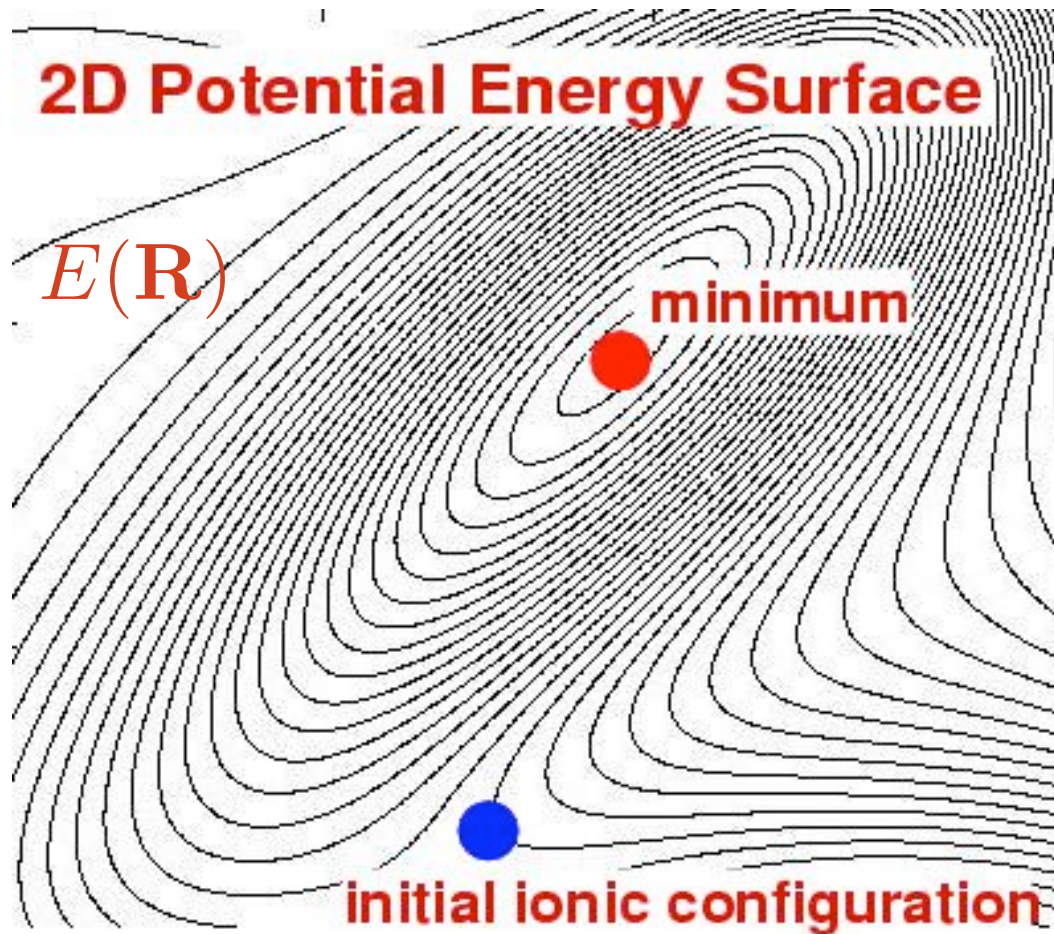


US pseudopotentials



$$H_{US}\phi_n = \epsilon_n S\phi_n \quad \langle \phi_n | S | \phi_m \rangle = \delta_{nm}$$

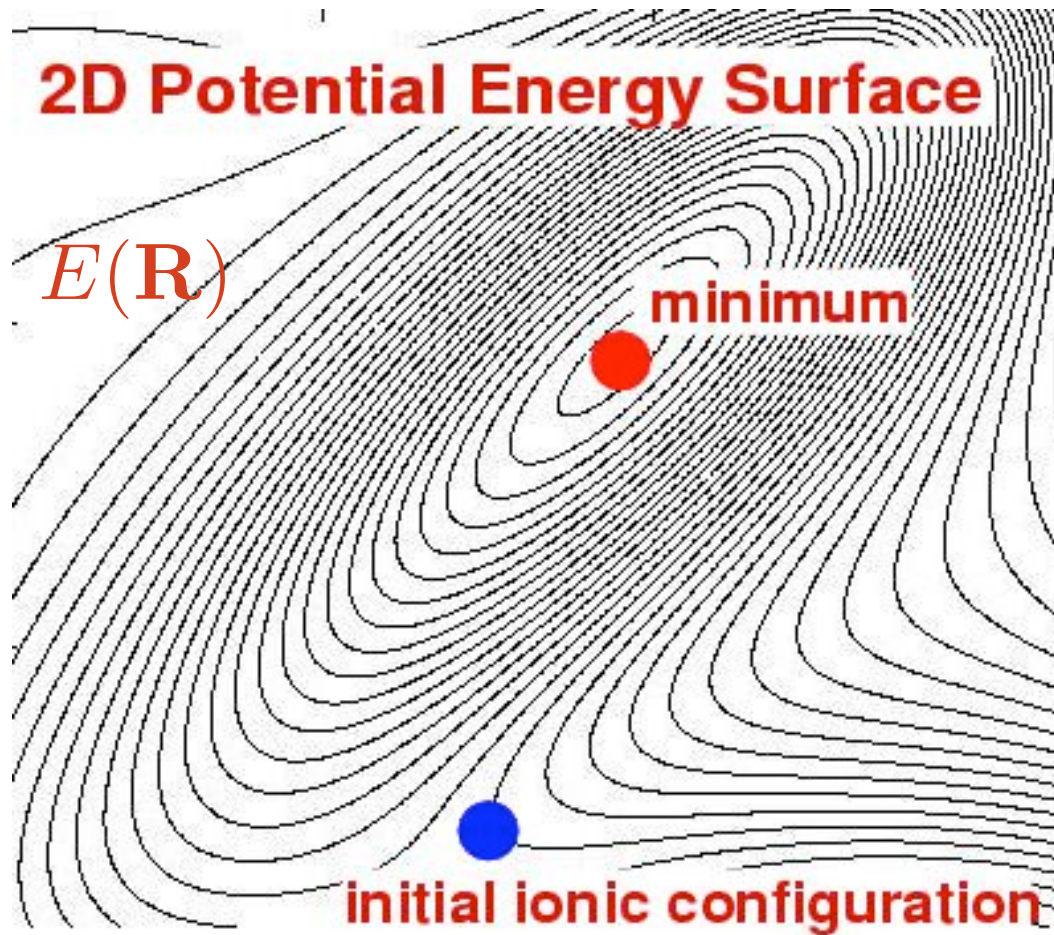
Structural optimisation



Equilibrium geometries:
minimum-energy
configurations

$$\mathbf{F}(\mathbf{R}) = -\frac{\partial E(\mathbf{R})}{\partial \mathbf{R}} = 0$$

Structural optimisation



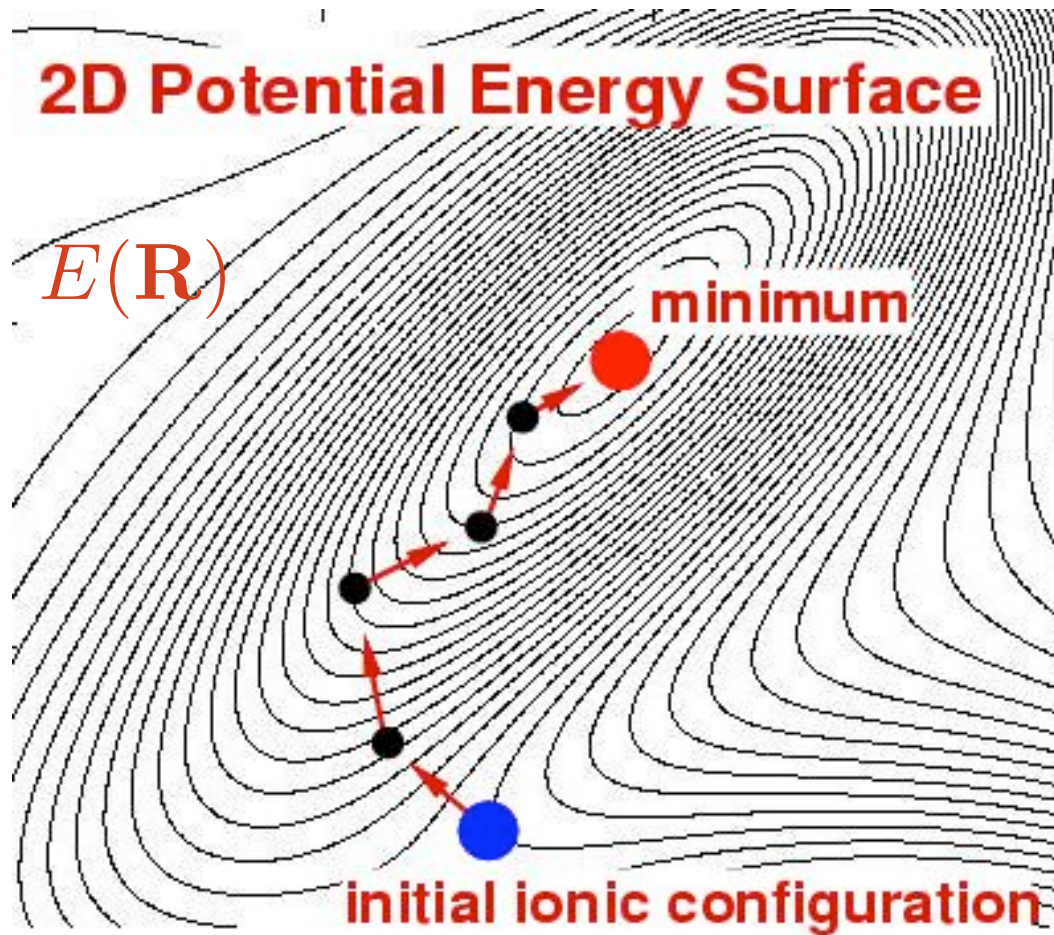
steepest descent

$$\dot{\mathbf{R}} = \mathbf{F}(\mathbf{R})$$

discretization

$$\mathbf{R}_n = \mathbf{R}_{n-1} + \epsilon \mathbf{F}(\mathbf{R}_{n-1})$$

Structural optimisation



The minimum is reached !!!

steepest descent

$$\dot{\mathbf{R}} = \mathbf{F}(\mathbf{R})$$

discretization

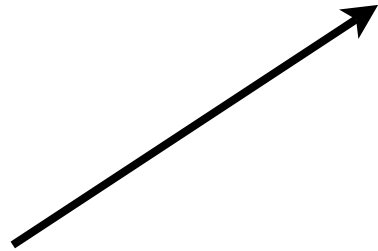
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Molecular Dynamics

$\mathbf{R}(t)$

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$\mathbf{R}(t)$



dynamics,
spectroscopy

Molecular Dynamics

$\mathbf{R}(t)$

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$$\langle A \rangle \approx \frac{1}{T} \int_0^T A(\mathbf{R}(t)) dt$$

Equilibrium
statistical mechanics

The Verlet algorithm

$$\mathbf{R}(t \pm \epsilon) = \mathbf{R}(t) \pm \epsilon \dot{\mathbf{R}}(t) + \frac{\epsilon^2}{2} \ddot{\mathbf{R}}(t) \pm \frac{\epsilon^3}{8} \dddot{\mathbf{R}}(t) + \mathcal{O}(\epsilon^4)$$

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$$\langle A \rangle \approx \frac{1}{N} \sum_{n=1}^N A(\mathbf{R}_n)$$

The tricks of the trade

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- Plane waves require supercells for treating finite (or semi-infinite) systems

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- ...and many others (and you got to know them all!)

Accuracy vs. approximations

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Theoretical approximations / limitations

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Theoretical approximations / limitations

- The Born-Oppenheimer approximation

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- ? Dispersion forces / weak chemical bonds

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The Quantum ESPRESSO suite of ab-initio codes

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*opEn Source Package for Research in
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Utilities and/or graphical applications

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is a community enterprise

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but rather what you can do for Quantum ESPRESSO

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- ✓ Be part of the community

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- ✓ Be part of the community
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To start with ...

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Enjoy this
course!

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