Early impact of quantum physics on chemistry: George Hevesy's work on rare earth elements and Michael Polanyi's absorption theory

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Theoretical chemistry or applied physics

reductionism

Paul Dirac:
„The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, ad the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.” (1929)

quantum chemistry

- VB theorists:
  - Walter Heitler (1904-1981), Fritz London (1900-1954), John C. Slater (1900-1976), Linus Pauling (1901-1994)
- MO theorists:
  - Friedrich Hund (1896-1997), Robert Mulliken (1896-1986)

The discovery of hafnium

standard history

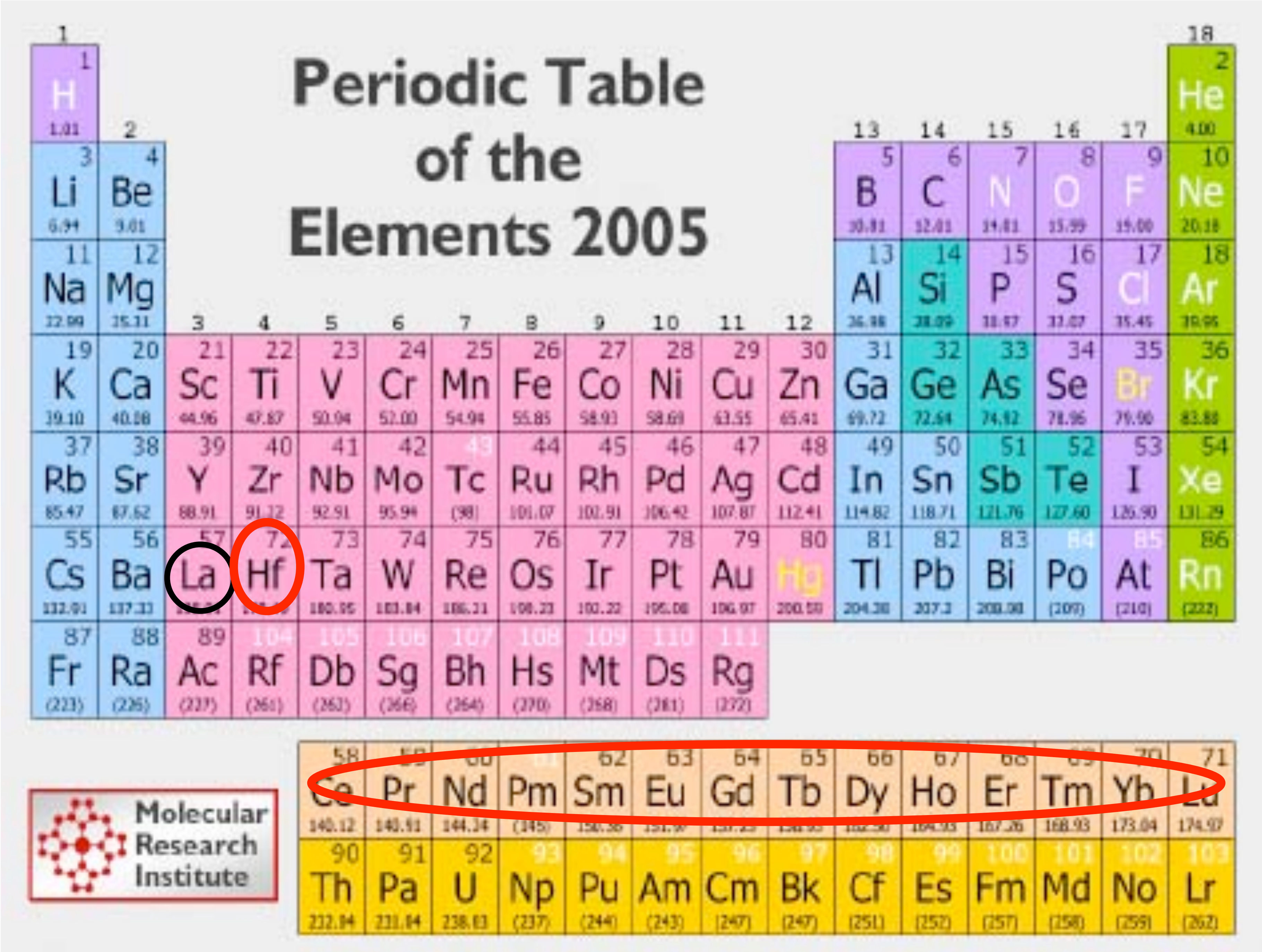
Encylopeadia Britannica : “Bohr pointed out that the missing element 72 would be expected, from its position in the periodic system, to be similar to zirconium in its properties rather than to the rare earths; this observation led G. de Hevesy and D. Coster in 1922 to examine zirconium ores and to discover the unknown element, which they named hafnium.”

reductionism

Karl Popper:
“it [the discovery of hafnium] struck us then as the great moment when chemistry had been reduced to atomic theory.” (1988)

electron configuration of the atoms

No.	Element	K	L	M	N	O	P
56	Barium	2	8	18	18	8	2
57	Lanthanum	2	8	18	18	9	2
58	Cerium	2	8	18	19	9	2
59	Praseodymium	2	8	18	21	8	2
60	Neodymium	2	8	18	22	8	2
61	Promethium	2	8	18	23	8	2
62	Samarium	2	8	18	24	8	2
63	Europium	2	8	18	25	8	2
64	Gadolinium	2	8	18	25	9	2
65	Terbium	2	8	18	27	8	2
66	Dysprosium	2	8	18	28	8	2
67	Holmium	2	8	18	29	8	2
68	Erbium	2	8	18	30	8	2
69	Thulium	2	8	18	31	8	2
70	Ytterbium	2	8	18	32	8	2
71	Lutetium	2	8	18	32	9	2
72	Hafnium	2	8	18	32	10	2
73	Tantalum	2	8	18	32	11	2



Periodic Table
of the
Elements 2005
1 H 2 He
3 Li 4 Be 5 B 6 C 7 N 8 O 9 F 10 Ne
11 Na 12 Mg 13 Al 14 Si 15 P 16 S 17 Cl 18 Ar
19 K 20 Ca 21 Sc 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr
37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53 I 54 Xe
55 Cs 56 Ba La 73 Ta 74 W 75 Re 76 Os 77 Ir 78 Pt 79 Au 80 Hg 81 Tl 82 Pb 83 Bi 84 Po 85 At 86 Rn
87 Fr 88 Ra 89 Ac 104 Rf 105 Db 106 Sg 107 Bh 108 Hs 109 Mt 110 Ds 111 Rg
Pr Nd Pm 62 Sm 63 Eu 64 Gd 65 Tb 66 Dy Ho Er Tm Yb 71
90 Th 91 Pa 92 U 93 Np 94 Pu 95 Am 96 Cm 97 Bk 98 Cf 99 Es 100 Fm 101 Md 102 No 103 Lr
Molecular
Research
Institute

Georges Urbain

- Chemist, 1872 - 1938
- Professor of inroganic chemistry at Sorbonne
- discovered lutetium

Georges de Hevesy

- chemist, 1885 - 1966
- Copenhagen, Freiburg, Stockholm
- radioactive tracers, hafnium, neutron activation analysis
- Chemistry Nobel Prize, 1944

Scanned at the American Institute of Physics

The theory of adsorption

Michael Polanyi

- Physician, chemist, philosopher, 1891 - 1976
- Budapest, Berlin, Manchester,
- Roentgen crystallography, theory of adsorption, reaction kinetics, philosophy

Polanyi's formula for adsorption potential

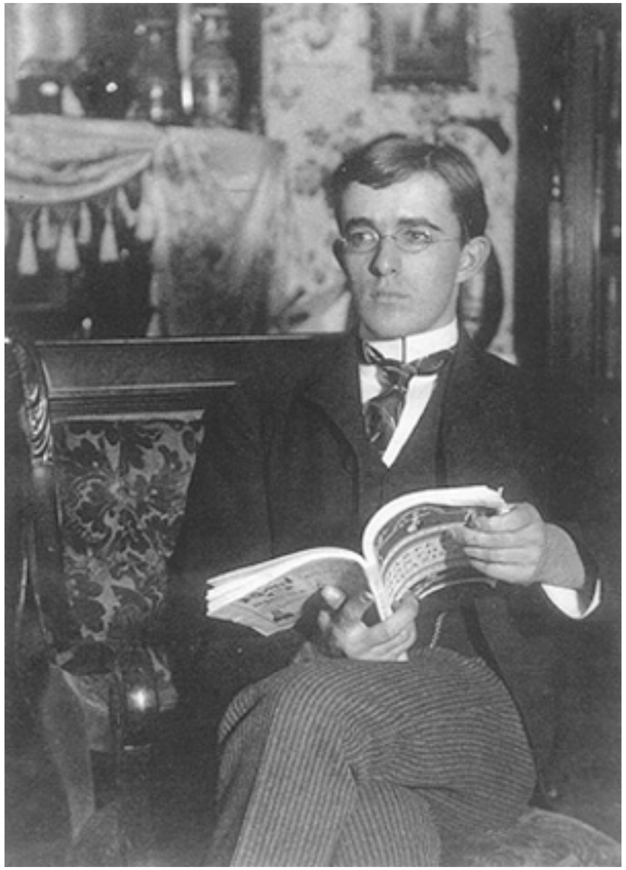
$$\varepsilon = f(\varphi)$$

ε is adsorption potential

φ is space above the adsorbent

Irving Langmuir

- Physicists, chemist, 1881 - 1957
- USA, Research Laboratory of the General Electric Company at Schenectady
- Theory of chemical bond, adsorption, incandescent light bulb, atmospheric science,
- 1932, Chemistry Nobel Prize



Fritz London

- physicist, 1900 - 1954
- Munich, Zurich, Berlin, Oxford, Paris, USA Duke Univ.
- quantum physics, quantum chemistry, superfluity, superconductivity

Dispersion force

$$E_{AB}^{\text{disp}} \approx -\frac{3\alpha^A \alpha^B I_A I_B}{2(I_A + I_B)} R^{-6}$$

A and B two atoms
$\forall^A$ and $\forall^B$ are the dipole polarizabilities
IA and IB are the first ionization potentials
R is the intermolecular distance

dispersion force above the adsorbent

From the two-molecule formula

c/r^6

one can derive the attraction to a surface formula

ε **$= Nc/6d^3$**

where d is the perpendicular distance from surface to molecule

Polanyi’s letter to a friend

“Whose fate is better, mine or Langmuir’s? My theory is absolutely right but not accepted. Langmuir’s theory is wrong but very famous... Langmuir is better off.”

Polanyi’s memory of his thory of adsorption

“my belief in my theory was quite unshaken...“ and he went on in this way “I became immune to these objections, but I remained powerless to refute them.”

Conclusions

- neither in the case of the discovery of hafnium, nor in adsorption theory were reduced chemistry quantum physics
- quantum physics had a heuristic and interpretative role in chemistry
- the two fields cooperated both intellectually and sociologically