

1 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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According to the standard history, the influence of quantum physics upon chemistry started in 1927. This was the publication year of Heitler and London's seminal article on the hydrogen molecule, an article that is supposed to have radically changed the theory of chemistry and endangered its independence.¹ Since then, many people have considered chemistry as a kind of applied physics, more precisely, of quantum physics. Meanwhile, to researchers working in less theoretical fields of chemistry, such as synthetic organic chemistry or classical chemical analysis, might have remained unnoticed that their discipline disappeared as it had been reduced to physics. In their eyes, chemistry seemed entirely different from physics, even if quantum physics exerted important impact upon its theoretical parts. In the followings, I will detail two cases of the early 1920s to show this impact. The underlying intention of this paper is to demonstrate the non-reductive heuristic value of quantum physics inside chemistry. I emphasize that 'inside chemistry' because the central characters of the two stories are not physicists but chemists, George von Hevesy and Michael Polanyi.²

The statement that Hevesy and Polanyi were not physicist but chemists, tacitly includes (to use Polanyi's phrase) that a sharp boundary existed between physics and chemistry, hence we can decide whether someone stands in one or the other side of the boundary. In a scrutiny, however, the boundary problem seems related to reductionism, to the questioned independent status of chemistry. After some general historical remarks on this issue, I will recapitulate the discovery of a chemical element, hafnium, and the interpretation of gas adsorption. The hafnium story is related to the old quantum theory while the absorption theory to quantum mechanics. In both cases, we will see fervent scientific controversies.

¹W. Heitler, F. London, "Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik. Zeitschrift für Physik. 44. 1927. 455–472.

²Some recent biographies of Hevesy and Polanyi: Siegfried Niese, Georg von Hevesy: Wissenschaftler ohne Grenzen. Dresden: Forschungszentrum Rossendorf, 2005. William T. Scott, Martin X. Moleski, S.J., Michael Polanyi: Scientist and Philosopher, Oxford: Oxford University Press, 2005.

Theoretical Chemistry or Applied Physics

Chemistry, and probably other disciplines too, has always had to carry on boundary works, to use Thomas Gieryn's term, meaning that it had to take efforts to demarcate its territory both from physics and biology.³ Looking back as far as to the 31st Query of Newton's *Optics*, or to the chemical revolution, chemistry's relation with physics has been uneasy.⁴ The boundary problem between physics and chemistry can be connected with physicalism, a positivist philosophical stand. In the 19th century, chemical concepts had been attempted to interpret in the framework of mechanics, thermodynamics or electricity. Concepts, such as affinity, valence, chemical bond, later spectroscopy, reaction kinetics, electrochemistry appeared to be very close to physical notions. In an ideal situation, the chemical concepts were assumed to be derivable from the first principles of theoretical physics. On the other hand, many fields of chemistry, including synthetic organic chemistry, were nearer to a particular laboratory practice than to an Aristotelian ideal of science relying on first principles.

Sociologically, the boundaries of chemistry were set by special jobs, by professional university departments providing degrees of chemistry, by textbooks, journals, scientific societies, highly admired researchers, professors, such as Lavoisier, Dalton or Berzelius and their scientific schools, by particular results and tenets like the periodic system created in 1869.⁵ By all these means, the discipline of chemistry defined a territory with boundaries worth defending and occasionally extending.

Quantum physics attacked the boundaries both of biology and chemistry. In his work titled *What is life*, Erwin Schrödinger initiated a research program aiming at explaining biological phenomena in a reductionist way, similarly to the way quantum physics explains microphysical phenomena.⁶ Max Delbrück and others became supporters of this program that brought major breakthroughs in biology.⁷

Quantum physics entered chemistry with Stark and Einstein's second law of photochemistry in 1912. The first fundamental results were achieved in 1913 by Niels Bohr's model of the atom, and his explanation of the periodic table, to which he returned in 1921–23.⁸ Although Bohr's theory was considered to be physics, chemists liked to use it

³Thomas Gieryn, *Cultural Boundaries: of Science: Credibility on the Line*. Chicago, London: Chicago University Press, 1999.

⁴A vast amount of literature discussed this problem. See, e.g., Evan M. Melhado, "Chemistry, Physics, and the Chemical Revolution," *Isis* 76. 1985. 195–211.

⁵Mary Jo Nye analyzed the general features of disciplines, mainly chemistry, through their identities. Mary Jo Nye, *From Chemical Philosophy to Theoretical Chemistry: Dynamics of Matter and Dynamics of Disciplines, 1800–1950*. Berkeley, Los Angeles, London: University of California Press, 1993.

⁶E. Schrödinger, *What is Life?* Cambridge: Cambridge University Press, 1944.

⁷In the vast literature see, e.g., D. Fleming, "Émigré Physicists and the Biological Revolution." In: D. Fleming, B. Bailyn, *The Intellectual Migration: Europe and America, 1930–1960*. Cambridge (Mass.): Harvard University Press, 152–189.

⁸N. Bohr, *On the Constitution of Atoms and Molecules* (Papers reprinted from the *Philosophical Magazine* with an introduction by L. Rosenfeld). Copenhagen and New York: Munksgaard and W. A. Benjamin. On the later results see N. Bohr, "The Structure of the Atom," (Nobel Lecture, December 11, 1922.) *Nobel Lectures, Physics, 1922–1941*. Amsterdam: Elsevier Publishing Company, 1965. About the extension of Bohr's building-up theory to molecules, see Buhm Soon Park, "A Principle written in Diagrams: The Aufbau Principle for Molecules and its Visual Representations. 1927–1932." In: U. Klein (ed.), *Tools and Modes of Representation in the Laboratory Sciences*, Dordrecht, Boston, London: Kluwer Academic Publishers, 2001. 179–98.

for interpreting chemical phenomena, because of the model's simplicity and because to a large extent it relied on chemical experimental data.

The radical reductionist program evolved after the introduction of quantum mechanics. In 1929, soon after the publication of Heitler and London's seminal article, Paul Dirac pronounced a radical reductionist program, saying that "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."⁹

Indeed, based on Heitler and London's initial ideas, Slater and Pauling with others established the so-called valence-bond theory, VB in 1927. Hund and Mulliken published the rival theory, called molecular orbital, MO, theory in the same year. In the VB method, hydrogen molecule was considered as an aggregate of two distinct hydrogen atoms, in which the two electrons constituting the chemical bond were placed between the two nuclei. The atoms were distinct physical systems and the theory described their connection. The MO theory, on the other hand, considered the hydrogen molecule as one physical system, having two electrons in one orbital around the two nuclei. The two approaches have competed in quantum chemistry for decades.¹⁰

Historians Ana Simoes and Kostas Gavroglu, however, pointed at another distinction. In the 1930s, Linus Pauling, a follower of Heitler and London's VB method, used the notion of resonance for explaining traditional organic chemistry problems, such as the tetravalency of carbon, the aromatic structure of benzene, the three-electron bond, and the like. By these, Pauling became part of the structural chemistry tradition rather than the tradition of theoretical physics. Simoes attributed this position partly to Pauling's ties with a research program initiated by Gilbert N. Lewis. Lewis suggested that the atoms composing a molecule could share electron pairs that secure the covalent bond between them. The other factor was a kind of pragmatism, manifested in the so-called 'semi empirical' method. This procedure combined theoretical, quantum physical calculations with empirical data of chemistry, instead of sticking to the physical goals of deriving chemistry from first principles. Simoes and Gavroglu argued that Pauling and Mulliken started a non-reductionist, chemistry-oriented version of quantum chemistry that was rooted in the American pragmatism.¹¹

No wonder: Lewis, Pauling and Mulliken were trained as chemists. If quantum chemistry was a fence at the boundary between physics and chemistry, Heitler and London, and most of their followers were sitting on the fence with legs toward physics, while Mulliken and Pauling with legs toward chemistry.¹²

⁹P.A.M. Dirac, "Quantum Mechanics of Many Electron Systems," *Proceedings of the Royal Society of London*, A123 (1929): 714–733, on 714

¹⁰On the history of quantum chemistry see Mary Jo Nye, ref. 5. p. 227–261.

¹¹A. Simões, "Chemical Physics and Quantum Chemistry in the Twentieth Century." In Mary Jo Nye (ed), *The Modern Physical and Mathematical Sciences. The Cambridge History of Science*, Vol. 5. Cambridge: Cambridge University Press, 2003. 394–412., A. Simões, K. Gavroglu, "Issues in the History of Theoretical and Quantum Chemistry, 1927–1960." In: C. Reinhardt (ed.), *Chemical Sciences in the 20th Century*. Weinheim: Wiley-VCH, 2001., and K. Gavroglu, A. Simões, "The Americans, the Germans, and the beginnings of quantum chemistry: The confluence of diverging traditions." *Historical Studies in the Physical Sciences*, 25(1), 1994, 47–110.

¹²Buhm Soon Park emphasized that quantum chemistry gradually put on a technical, computational character with a diminishing physical relevance. Buhm Soon Park, "Computational Imperatives in Quantum Chemistry," Paper presented at the HQ-1 conference, July 2–6, 2007, Berlin.

The Discovery of Hafnium

Encyclopaedia Britannica presented the standard history of the hafnium's discovery as follows: "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."¹³

In this account, Bohr's theory concerning the periodic table was corroborated by Hevesy and Coster. This presentation of the story follows the logic of a reductionist and Popperian philosophy. Indeed, Popper wrote: "all attempts to find it [the chemical element with atomic number 72] were in vain until Bohr succeeded in predicting several of its properties by deducing them from his theory."¹⁴ At another place, Popper said that "it [the discovery of hafnium] struck us then as the great moment when chemistry had been reduced to atomic theory."¹⁵

From Bohr's point of view, the problem was that while working on the electronic building-up of the atoms in the periodic system, he had to place the still unknown element 72 somewhere in the periodic system. He faced with the dilemma whether the this element was a rare earth to be placed in a separate row below the table with the other rare earths or it was a transition metal to be placed on the table. From his theory, Bohr concluded that element 72 was a transition metal because of its electronic structure.

In his method, by proceeding forward in the periodic table to successive atoms an extra electron should be added to the previous ones. The electrons were arranged in shells and outer shell received the next coming electron. Arriving at the element 57 (see Table ??), lanthanum, however, the electrons did not continue to fill the outer *P* shell. Instead, the added electron was placed on the inner *O* shell, *5d*, and in the following elements, starting with cerium, the *N* shell, *4f*, were built up, while the *O* and *P* shells remained unchanged. Fourteen electrons fulfilled the *4f* shell. Hence, the last element belonging to this group should be 71, lutetium, because 57 (element number of lanthanum) + 14 = 71. The configuration of the outer shell determines the chemical properties of the elements. Since the outer shell of the elements 57 – 71 did not change, only inner shells changed, the chemical properties of these elements should be almost identical. These are the rare earth elements. After the *4f* shell has been fulfilled at element 71, the next electron goes to the *O* shell, *5d*, again, making the properties of the unknown element 72 different from the previous ones. Therefore, element 72, should not be a rare earth, and it should be placed on the main table with the transition metals.

From chemical point of view, the historical process seemed different, because the logic of chemical research on rare earths was influenced by the changing methods of analytical chemistry, rather than physical ideas. As historian of analytical chemistry, Ferenc Szabadváry pointed out, rare earths were found mainly in two minerals, yttria and ceria. The chemical properties of rare earths proved almost identical with each other. Moreover, they occurred together in these two minerals. Hence, to separate them (that started in 1787) was extremely difficult and uncertain. This is why their discovery fol-

¹³[HTTP://WWW.BRITANNICA.COM/NOBELPRIZE/ARTICLE-80831](http://www.britannica.com/nobelprize/article-80831)

¹⁴K. Popper, *The Logic of Scientific Discovery*. London: Hutchinson, 1959. p. 69.

¹⁵K. Popper, *The Open Universe*. London: Hutchinson, 1982. Cited by Eric Scerri, "Popper's Naturalized Approach to the Reduction of Chemistry," *International Studies in the Philosophy of Science*, 12. 1998. 33-44. p. 34.

Early Impact of Quantum Physics on Chemistry: Hevesy and Polanyi

Number	Element	<i>K</i>	<i>L</i>	<i>M</i>	<i>N</i>	<i>O</i>	<i>P</i>
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

Table 1.1: Electron configuration of some atoms.

lowed a pattern of division: some components were held to be new chemical elements, but subsequently they proved to be mixtures, the components of the mixture were thought to be elements, but one of them proved to be a mixture, and so on. For instance, in 1905, Auer von Welsbach, an Austrian chemist, applied fractional crystallization of the double oxalates and found out that an element called ytterbium was in fact a mixture of two elements. The French professor Georges Urbain used his own method, based on a ‘separating element’ that crystallizes with rare earth elements, and came to the same conclusion. They simultaneously discovered element 71, lutetium. Chemists found new and new rare earth elements and their final number was uncertain. In 1911, Urbain announced to find a new element mixed with lutetium. He called it celtium, the element 72, another rare earth. In 1922, Urbain with a co-author confirmed the existence of celtium by Roentgen spectroscopy.¹⁶

This confirmation caused severe headache to Bohr, who wanted to present his new interpretation of the periodic system in his Noble lecture in 1902. He explained the problem to his friend, George de Hevesy, a chemist working in the Bohr institute. Supposing that element 72 was homologue with zirconium, Hevesy with his colleague, the physicist Dirk Coster, analyzed a Norwegian zirconium mineral, by Roentgen spectroscopy and found the unknown element number 72, subsequently named hafnium. Hevesy separated hafnium and proved that it had no rare earth chemical properties.¹⁷

¹⁶Ferenc Szabadváry, “The History of the discovery and Separation of the Rare Earth,” In K. A. Gschneider, Jr., L. Eyring, Handbook of the Physics and Chemistry of Rare Earths, Vol. 11. Amsterdam: Elsevier Science Publisher, 1988. 33–80.

¹⁷Hevesy told this story many times, including his biographical notes that were published with insignificant corrections by J. D. Cockroft as an obituary of Hevesy. J. D. Cockroft: “George de Hevesy

The result of this controversy¹⁸ seems to prove the advantage of the physical theory over chemical experimenting. Karl Popper referred to the hafnium story in this context. More recently, however, philosopher Eric Scerri has challenged the reductionist analysis in a non-reductionist framework. His interpretation of hafnium's discovery relies on two arguments. According to the first one, Bohr's model was not a logical precondition for listing element 72 among transition metals. Some chemists, including the Danish Thomsen in 1895, predicted that element 72 would be homologous with zirconium. After knowing the results of Moseley's Roentgen spectroscopy measurements carried out in 1914, this place appeared doubtless. According to the other argument, which seems stronger in our context, the discovery of hafnium does not support reductionism, because the Bohr model itself was not a deductive result from first principles. Scerri argued that this model, the old quantum theory was inductive relying on various experimental facts, many originating in chemistry.¹⁹

Indeed, in the tradition of chemistry, the discovery of hafnium is attributed to George Hevesy, a chemist. This exemplary case neither proves, nor falsifies the potential reduction of chemistry to physics but demonstrates an effective collaboration between quantum physics and chemistry.

Theory of Adsorption

Adsorption is a phenomenon whereby gasses are attracted and stuck to the surface of a solid. Michael Polanyi did pioneering but controversial research on adsorption. His ideas might originate in the biographical contingency that Polanyi graduated from medicine, obtaining limited training in chemistry. He worked out the basic elements of his potential theory of adsorption, while being hospitalized in Budapest, in 1914, without any access to the current scientific literature.²⁰

As he did not know about the electronic theory of chemical processes, Polanyi based his interpretation of adsorption on classical thermodynamics. He thought that the van der Waals type attractive forces originated in the surface of solids establish a potential gradient. Polanyi called this force adsorption potential, and assumed that it influenced the gas above the adsorbent in a way that was similar to compression. By the work done by adsorption potential, the gas was thought to condense in an adsorbed phase upon the surface of the solid. Adsorption potential was defined by a simple formula: $\varepsilon = f(\varphi)$, in which ε is the adsorption potential, φ is the space where the force is effective. In this model, the adsorbed layers of gas were several molecules thick.²¹

1885–1966”, Biographical Memoirs of Fellows of the Royal Society, 13. 1967, 125–166. D. Coster, G. Hevesy, “On the new element hafnium.” *Nature*, 111. 1923. 182, and 252. After working out the details of the hafnium chemistry, Hevesy published a monograph on the new element: G. Hevesy, *Das Element Hafnium*. Berlin: Springer, 1927.

¹⁸About the controversy, see H. Kragh, “Anatomy of a priority conflict: The case of element 72.” *Centaurus*. 23. 1980. 275–301.

¹⁹E. Scerri, “Prediction of the Nature of Hafnium from Chemistry, Bohr’s Theory and Quantum Theory.” *Annals of Science*. 51. 1994. 137–150.

²⁰About Polanyi’s life, see W. T. Scott, M. X. Moleski, S.J. , *Michael Polanyi: Scientist and Philosopher*. Oxford: Oxford University Press, 2005.

²¹M. Polanyi, “Adsorption, Quellung und osmotischen Druck von Kolloiden,” *Biochemische Zeitschrift*, 66. 1914. 258–268., M. Polányi, “Über Adsorption und Kapillarität vom Standpunkte des II. Hauptsatzes,” *Zeitschrift für physikalische Chemie*, 88. 1914. 622–631., M. Polanyi, “Über die Adsorption

This consequence of Polanyi's potential theory of adsorption met serious disagreements. In 1921, living already in Germany, Polanyi was invited to give an account of his theory at the seminar of the Kaiser-Wilhelm Institute for Physical Chemistry and Electrochemistry.²² Characteristically, the chemist audience, including Herbert Freundlich, head of department and expert of adsorption, or Hermann Mark, found Polanyi's theory convincing because it was in harmony with the experimental data available then.²³ However, Haber, Nernst and particularly the special guest, Albert Einstein strictly refused it. "I survived the occasion only by the skin of my teeth."—Polanyi remembered in 1963.²⁴

The attack was directed against the multimolecular layers of the adsorbed molecules on the adsorbent. The critics thought it was impossible for two reasons. Firstly, because Polanyi had no convincing theory on the nature of the attractive force originated in the surface of the adsorbent. His thermodynamic argumentation was considered old fashioned, which disregarded contemporary results of physics related to the electronic character of the atomic and molecular forces, in particular, disregarded the nature of the dipole interactions. The critics supposed that the van der Waals type forces decreased by an inverse sixth power and that the dipole-dipole forces between the adsorbed molecules were shielded out by the adsorbed molecules. They did not see any force to keep several layers of the adsorbed molecules on the surface of the adsorbent.²⁵

Secondly, the criticism referred to Polanyi's negligence of Irving Langmuir's adsorption theory that was launched in 1916 and gradually became main stream. Langmuir relied on the latest physical theories, including electronic structure of matter, electron pairs and chemical bond. In his adsorption theory, Langmuir supposed that electrostatic forces originate in the adsorbent, which are related to the valence of the molecules on the surface of the adsorbent. Because of the range of this force, the gas molecules can only constitute a monomolecular layer on the surface of the adsorbent. Langmuir published an isotherm equation, the widely used Langmuir isotherm, and supported his theory by elegant experimental results. Polanyi's rival proved so persuasive that he received the 1932 Chemistry Nobel Prize.²⁶

In spite of Einstein and Haber's criticism and Langmuir's success, Polanyi was convinced about the value of his theory, even if was based on a 19th century physical picture. His supposedly victorious argument came from quantum theory. Fritz London,

vom Standpunkt des dritten Wärmesatzes," Verhandlungen der deutschen physikalischen Gesellschaft, 16. 1914. M. Polányi: Adsorption von Gasen (Dampfen) durch ein festes nichtflüssiges Adsorbens. Verhandlungen der deutschen physikalischen Gesellschaft, 18. 1916. 55–80. 1012–1016. Polanyi's PhD Theses: Polányi Mihály, Gázok (gozök) adsorbtiója szilárd, nem illanó adsorbensen. Doktori disszertáció. 30 o. Budapest, 1917.

²²About Polanyi's times in Berlin see Mary Jo Nye, "Historical Source of Science-as-a-social-practice: Michael Polanyi in Berlin," *Historical Studies in the Physical and Biological Sciences*, 37. 2. 2007. 409–434.

²³The chemists' favorable reaction was reported in an interview with Hermann Mark. W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 74.

²⁴M. Polanyi, "The Potential Theory of Adsorption", *Science*, 141. 1963. 1010–3. Reprinted in: M. Polanyi, *Knowing and Being*. London: Routledge & Kegan Paul, 1969. p. 97–104.

²⁵W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 73.

²⁶Langmuir's fundamental paper: I. Langmuir, "The adsorption of gases on plane surfaces of glass, mica and platinum", *Journal of the American Chemical Society*, 40. 1918, 1361–1403. A wider view: I. Langmuir, "Surface chemistry", Nobel Lecture, December 14, 1932. [HTTP://NOBELPRIZE.ORG/NOBEL-PRIZES/CHEMISTRY/LAUREATES/1932/LANGMUIR-LECTURE.HTML](http://nobelprize.org/nobel_prizes/chemistry/laureates/1932/langmuir-lecture.html)

one of the physicist founders of quantum chemistry, after moving to Berlin at the end of the 1920s, regularly participated in the seminars at Haber's institute. By then Polanyi was a leading researcher of the institute, the head of a section, out of two sections of the institute. (The other section's head was Herbert Freundlich, chemist, an expert of adsorption.) In 1930, London published a quantum mechanical calculation on a weak force, called dispersion force, working between two dipoles.²⁷ From Polanyi's point of view dispersion force had two particularly important features. Firstly, it was not electric, therefore, shielding out does not occur. Secondly, its range above the adsorbent decreased by an inverse third power, rather than sixth powers as in the case of the van der Waals type forces, meaning that the range of dispersion force was much larger than the range of the van der Waals force. It seemed large enough to create more than one layers on the surface of the adsorbent. Polanyi cooperated with London in calculating the dispersion force working in the case of adsorption and they could identify dispersion force with Polanyi's adsorption potential, just the way he described in his study it in 1914 and 1916.²⁸ With his collaborators in Haber's institute, mainly H. Goldman, Polanyi created an apparatus for experimental research of adsorption by which they thought they confirmed the potential theory and the multilayer image of adsorption.

According to William Scott, Polanyi's biographer, in the early 1930s Polanyi felt great satisfaction seeing his original theory of adsorption to be justified.²⁹ Historian Mary Jo Nye added that in 1932, Polanyi's colleague, Herbert Freundlich published a paper intending to compromise between the two rival theories. Polanyi thought that Langmuir's formula was a simplistic idealization that can be derived as a special case from his theory. Although he thought that his theory was firm and well founded, Polanyi knew that it did not gain wide acceptance.³⁰ Scott cited a letter written by Polanyi 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." ³¹

Polanyi fled to Britain from Hitler in 1933, and gradually changed from chemistry to philosophy. In 1958, he published *Personal knowledge*, a very influential book on the philosophy of science inspired by cultural, moral, political and of course scientific commitments.³² Indeed, commitment was one of Polanyi's central categories besides tacit knowledge, focal and subsidiary awareness and others. All these served as conceptual instruments to analyze discoveries, rather than justification, unlike the main stream contemporary philosophy of science that divided scientific research between the context of justification and discovery. Discovery was considered contingent, psychological, and sociological, an inappropriate subject for rational philosophical reflections. Polanyi thought

²⁷F. London, "Theorie und Systematik der Molekularkräfte," *Zeitschrift für Physik*, 63. 1930. 245–279., F. London, "Properties and applications of molecular forces", *Zeitschrift für Physikalische Chemie (B)*, 11. 1930. 222–251. R. Eisenschitz, F. London, "Über das Verhältnis der van der Waalsschenkräfte zu den homoopolaren Bindungskräften," *Zeitschrift für Physik*, 60. 1930. 491.

²⁸F. London, M. Polanyi, "Über die atomtheoretische Deutung der Adsorptionskräfte," *Die Naturwissenschaften*, 18. 1930. 1099–1100.

²⁹W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 126.

³⁰Mary Jo Nye, "Michael Polanyi's Theory of Surface Adsorption: How Premature?," In: E. B. Hooke (ed.), *Prematurity in Scientific Discovery: On Resistance and Neglect*. Berkeley: University of California Press, 2002. 151–164.

³¹W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 112.

³²M. Polanyi, *Personal Knowledge*. London: Routledge and Kegan Paul, 1958; Chicago: Chicago University Press 1958.

that scientific ideas were born before research, as a kind of preliminary knowledge or belief, and research in fact articulates, justifies the ideas instead of producing them. Therefore, the precondition of a good research work is to believe in an idea that emerges in the course of doing science. His whole philosophy was about and based on belief and commitment whether speaking about science, epistemology, ethics, religion, or esthetics.

Although Polanyi worked out his philosophy several decades later than he had received criticism from his peers concerning his potential theory of adsorption, one cannot resist thinking that his behavior was motivated by his deep belief in and commitment to the multilayer model. When working it out, he was a young researcher, just left his country behind, lacking any shelter, any family or colleagues network, working on a field, physical chemistry, without proper basic training and receiving sharp criticism from leading experts of science. Polanyi needed that strong belief and commitment to his belief for not giving up, not fleeing from science. He was looking for justification. In 1963, remembering his adventure with the potential theory of adsorption, Polanyi wrote in *Science* that after the criticism he had received “my belief in my theory was quite unshaken...”.³³ He continued in this way: “I became immune to these objections, but I remained powerless to refute them.”³⁴ Eugen Wigner, Polanyi’s student had a different impression. He thought even Polanyi might have some doubts concerning his own theory of adsorption: “The writer of these lines [Wigner] remembers that when he pointed to some experimental data strongly supporting the multilayer character of adsorption, Polanyi was quite taken aback.”³⁵

According to Mary Jo Nye, by 1930 after about twenty years research work “the old-fashioned potential gradient now had a firm theoretical basis in the new quantum mechanics.”³⁶ By that time, however, the Langmuir approach rooted deeply in physical chemistry. Nevertheless, potential theory of adsorption stayed alive. Both Mary Jo Nye and William Scott showed that the theory found its way in the textbooks of chemistry. I can add that in the 1950s and 60s, the Hungarian physical chemistry and colloid chemistry textbooks also contained detailed descriptions of it with modernized versions, including that of M. Dubinin.³⁷ Multilayer adsorption theory has finally been accepted in the main stream.

Conclusions

The two cases, the histories of the discovery of hafnium and the potential theory of adsorption did not exemplify the reduction of chemistry to physics, although in both cases quantum physics played a crucial role. In both cases, chemistry seemed helpless in deciding controversial issues. A renowned authority in the field of rare earth chemistry,

³³M. Polanyi, “The Potential Theory of Adsorption”, ref 23. p. 89.

³⁴Ibid. p. 91.

³⁵E. P. Wigner, R. A. Hodgkin, “Michael Polanyi, 12 March 1891 – 22 February, 1976,” *Biographical Memoirs of Fellows of the Royal Society*, 23. 1977. 412–448.

³⁶T. Erdey-Gruz, G. Schay, *Elméleti Fizikai Kémia (Theoretical Physical Chemistry)*, Budapest: Tankönyvkiado, 1952–1954. The potential theories of adsorption are discussed (in the fourth edition published in 1964) in Vol. 2. p. 389–400. E. Wolfram, *Kolloidika*, (lecture notes for chemistry students of the Eötvös Lorand University) Budapest: Tankönyvkiado, 1965. p. 156–159.

³⁷Mary Jo Nye, “At the Boundaries: Michael Polanyi’s Work on Surfaces and the Solid State,” In: C. Reinhardt (ed.), *Chemical Sciences in the 20th Century*. Weinheim: Wiley-VCH, 2001. p. 249.

George Urbain concluded that element 72 was a rare earth, while some other chemists thought it was not. None of the arguments were entirely convincing to the chemical community that inclined to accept Urbain's position concerning cerium. Bohr's quantum theory was not considered decisive for chemists. However, Bohr's theory provided strong arguments to Hevesy to search for hafnium in a non rare earth mineral. In chemistry, the preparation of the new element counted as the strongest argument for the existence of this element, and the derivation from the first principles of physics did not matter very much. Bohr's model was not an attack against the border of chemistry, rather a useful heuristic instrument that helped chemists to interpret chemical phenomena, even after the model proved fallacious.

The history of adsorption showed some similar features. In working out his potential theory, Polanyi relied on the classical thermodynamics used by physical chemistry that he learned in Budapest mainly from Walter Nernst's book, *Theoretical Chemistry*.³⁸ Polanyi's approach was criticized referring to a pre-quantum mechanical view of molecular forces. Polanyi's adsorption potential gained solid theoretical foundation from quantum physics, sixteen years after its construction. However, in this case, foundation did not mean a deduction from first principles. The disadvantage of Polanyi's theory was that it failed to produce an equation for adsorption isotherms. Such a formula would have been considered a real analytical approach in the sense of physicalism. Adsorption has not been deduced from quantum physics or quantum chemistry, but it could be interpreted by it. Consequently, potential theory of adsorption remained behind the boundaries of physical chemistry, while it needed the quantum theoretical interpretation.

Our two cases revealed that quantum physics could play important role in chemistry without completely reducing it to physics. Sociologically, this was expressed by the cooperative efforts in our cases. Simoes and Gavroglu described the differences between the early German and American quantum chemistry schools in terms of the main character's relationship with chemistry, finding that the German quantum chemistry community consisted of physicists, while the Americans of chemists.³⁹ Our cases showed that in the European continent, including Germany fruitful cooperation was established between the two fields. In the case of hafnium, the chemist Hevesy cooperated with the physicist Bohr, in adsorption theory the chemist Polanyi with the physicist Fritz London. The representatives of the two disciplines walked to the boundary from two different directions and proceeded together peacefully along the border without any sorrow fight.

³⁸W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 25. Probably, it was an edition of Walther Nernst, *Theoretische Chemie vom Standpunkte der Avogadro'schen Regel und der Thermodynamik*. Stuttgart: Verlag von Ferdinand Enke, 1st edition, 1893.

³⁹K. Gavroglu, A. Simões, "The Americans, the Germans, and the beginnings of quantum chemistry: The confluence of diverging traditions," *Historical Studies in the Physical Sciences*, 25(1). 1994. 47–110.