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Theory in service of nanochemistry induced by electron impact

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The aim of this presentation is to show the recent progress in applications of quantum chemistry and theory of electron scattering to the needs of nanofabrication of chips by deposition of metallic structures on the surface. Over the past decade, a new method called Focused Electron Beam Induced Processing has gained increasing attention as a fast and versatile lithography with sub-5 nm features. However, the advantages of FEBID, such as high spatial resolution and accessibility, are currently overset by insufficient control of the purity and shape of the desired end product. If control of the process is to be improved, it is necessary to understand the parameters that dominate electron-induced chemistry. Here comes the help from the side of theory. We can calculate the cross sections for dissociative electron attachment, i.e., the probabilities of metal-ligand bond fission on electron impact, and consequently to predict suitable precursors and optimum electron energies. The calculations are based on the *ab inito* treatment of the Lippmann-Schwinger equation for vibrationally inelastic scattering and a quantum-chemical approach for a direct evaluation of dissociative attachment by a local resonance model. Possible benefits for general quantum chemistry will also be noted: use of graphics processing units, use of hybrid gaussian and plane-wave basis sets, and efficient evaluation of two-electron exchange integrals.

Biography

Petr Čársky has completed his PhD in 1968 from the Czechoslovak Academy of Sciences. He served two terms as the Director of Heyrovský Institute. Presently, he is continuing his work at Heyrovský Institute as a Senior Researcher. He has published more than 180 papers in reputed journals. He is a member of the International Academy of the Quantum Molecular Science and a WATOC board member, and has been serving as an Editorial Board Member of several reputed journals.

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