

Real-time description of fission

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Two major recent developments in theory and computational resources created the favorable conditions for achieving a microscopic description of nuclear fission almost eighty years after its discovery in 1939 by Hahn and Strassmann. The density functional theory (DFT) provides the only microscopic framework suitable for description of heavy nuclei and feasible on today's computers. Instead of computing the full many-body wave function, one can determine only the one-body density within the DFT, the highly successful approach pioneered by Kohn (Nobel prize, 1998), Hohenberg, and Sham (1964-1965) for many-electron systems in chemistry and condensed matter physics. Within the extension to time-dependent DFT, fission dynamics becomes computationally manageable and, hence, a microscopic description feasible. To study quantum dynamics we developed a real-time DFT extension, explicitly including the dynamics of the crucial pairing correlations, used existing reasonably accurate energy density functionals (EDF), and implemented it on leadership class computers. The current implementation allows us to obtain information about important aspects of the fission process, such as the particle emission during the fragment acceleration, or the excitation energy sharing between fragments, before neutron emission. For such observables, only indirect experimental information exists, but they are crucial in obtaining a good description of the emission of neutrons and gamma-rays from de-exciting fragments. Thus, even if no complete process description can be achieved yet (e.g. no neutron and gamma-ray emissions from fission fragments, which require very long evolution times), the information provided by the dynamics can be used as input into phenomenological Hauser-Feshbach codes that treat the de-excitation of fission fragments.

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