Ab initio simulation of ion stopping in strongly correlated materials

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The interaction of ions with solid surfaces is of crucial importance for many technological applications, in particular for nonideal plasmas. Ion stopping has been computed for a long time, and there exist many analytical models and code packages. However, these approaches typically neglect correlation effects in the solid material. We have recently developed first-principle simulations that are based on Nonequilibrium Green functions (NEGF) within an Ehrenfest approach for the ion [1]. First NEGF results for ion stopping were presented in Ref. [2]. Here we compare these results to time-dependent density functional simulations. Furthermore we present results of a recent extension of the NEGF simulation to a study of a special correlation effects: the ion-induced doublon formation in graphene-type nanoclusters [3]. Doublons are doubly occupied lattice sites in strongly correlated materials and have an important effect on the electronic properties and conductivity of these materials. Here we show that ion impact can effectively induce doublons giving rise to interesting applications.

REFERENCES

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