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UNIVERSITÄT DUISBURG ESSEN

Open-Minded

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Simulations of excited electronic states in materials across time and length scales

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Developing accurate models of material responses to intense radiation is crucial for radiation-resistant materials and materials manipulation at the atomic level. These models must account for rapid quantum interactions immediately post-irradiation, linking initial excited states to longer-term effects. In this talk I will present my group's work on describing such processes from first principles, with a particular focus on graphene, demonstrating that lattice temperature can significantly increase secondary electron emission compared to electronic heat. Our research points to very short emission pulses, offering tight temporal probing capabilities. Additionally, we are generalizing this approach towards cost-effective computational modeling: With little loss of accuracy, we train a machine learning model on high-fidelity quantum mechanical simulation data of electronic stopping to achieve a million-fold reduced computational cost, allowing for first-principles Bragg peak simulations. In the last part of this talk, I will discuss examples of how such simulations can make use of currently existing quantum computing hardware. My group explores simulations of ground and excited electronic states e.g. for oxygen vacancy defects near alumina surfaces, and we characterize and mitigate noise.

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

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