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Electronic correlation effects in the stopping power of ions in 2D materials LOTTE BORKOWSKI, FRANZISKA REISER, JAN-PHILIP JOOST, NICLAS SCHLÜNZEN, MICHAEL BONITZ, Kiel University — The energy loss of charged projectiles in correlated materials is of prime relevance for plasma-surface interaction for which we have developed a nonequilibrium Green functions (NEGF) approach. A particularly interesting effect is the *correlation induced increase* of stopping power at low velocities¹. However, NEGF simulations are possible only for short time durations, due to the unfavorable N_t^3 scaling with the number of discretization time steps. The situation has changed radically with the recently developed G1-G2 scheme², which is based on the generalized Kadanaoff-Baym ansatz in combination with Hartree-Fock propagators, and allows to *achieve linear scaling* with N_t . This enhancement enables us to improve previous simulations by using better selfenergies³, studying larger systems and by extending the simulation duration which gives access to slower projectiles. Finally, we will report further improvements of the G1-G2 scheme itself, by taking into account three-particle correlations.

¹Balzer *et al.*, *Phys. Rev. Lett.* **121**, 267602 (2018)

²Schlunzen *et al.*, *Phys. Rev. Lett.* **124**, 076601 (2020)

³Joost *et al.*, *Phys. Rev. B* **101**, 245101 (2020)

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