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First-principles simulation of laser irradiation of graphene and graphane[1] KALMAN VARGA, SERGIY BUBIN, Vanderbilt University — In the framework of real-time real-space time-dependent density functional theory complemented with classical molecular dynamics for ions, we have studied the behavior of graphene and graphane fragments irradiated with strong laser pulses. In particular, we have investigated how the response of graphene and graphane changes when laser pulses of different frequency (near IR, visible, and UV) are shot. Damage thresholds have been established and compared with existing experimental data.

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