Selective Defect Engineering in Two-Dimensional Materials: predictions from first-principles simulations

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We present a systematic investigation of displacement threshold energies in graphene and hexagonal boron nitride (h-BN) under low-energy ion-beam irradiation, covering 63 elemental projectiles from beryllium to mercury (excluding the lanthanides). This dataset establishes a broad foundation for controlled vacancy engineering and ion implantation in h-BN, with direct relevance to emerging quantum technologies including single-photon emitters and quantum sensors. Our ab initio molecular dynamics simulations reveal that chemical interactions between the incident ion and target atom dominate implantation and sputtering outcomes in the low-energy regime. While the classical binary collision approximation provides reasonable predictions for noble gases, it fails for elements that form strong transient bonds with the lattice. We further demonstrate a strong correlation between the displacement threshold energy and the vacancy formation energy when the ion approaches bonding distances. Building on these insights, we outline a strategy for selective sublattice displacement in binary compounds such as h-BN, and we identify which elements can be directly implanted by substituting specific lattice sites. Together, these results offer predictive guidance for atomic-scale defect engineering in two-dimensional materials.