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Chemically controlled dislocation migration in two-dimensional MoS_2 XIAOLONG ZOU, MINGJIE LIU, BORIS YAKOBSON, Department of Materials Science and NanoEngineering, Dept. of Chemistry, and Smalley Institute for Nanoscale Science and Technology, Rice University — As an additional Gibbs degree of freedom, chemical potential plays an important role in determining various properties of hetero-elemental two-dimensional (2D) materials, ranging from the equilibrium shape [1], to defect structures [2,3], electronic [3], and magnetic properties [4]. Here, by first-principles calculations, we demonstrate how the chemical potential control can be adopted as a feasible strategy to tune the dislocation dynamics in 2D MoS_2. Depending on the structures of the migrating dislocations, two different dynamic mechanisms are revealed, either through the direct *bond-rebinding (BR)* mechanism, where only single metal atom moves significantly, or *concerted migration (CM)*, in which case several atoms rearrange concurrently. The migration barriers for CM mechanism could be 2 to 4 times larger as the BR ones. Our detailed analyses show that under certain range of chemical potential some dislocations with high mobility could nevertheless also have quite high stability, which opens up the possibility of enhanced plasticity and suggests intriguing future applications.

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