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Using Defects in Materials to Store Energy: a Theoretical Study

I-TE LU, MARCO BERNARDI, Department of Applied Physics and Materials Science, California Institute of Technology — We study the energy stored by defects in materials using density functional theory (DFT) calculations. Leveraging experimental data to estimate the energy density of defects, expressed as the defect formation energy per unit volume (units of MJ/L) or weight (units of MJ/kg), we identify candidates for high energy density storage, including tungsten, diamond, graphite, silicon, and graphene. DFT calculations are applied to these materials to study the formation energy of vacancies, interstitials, and Frenkel pairs. Our results indicate that the energy density stored by defects in these materials, with experimentally accessible non-equilibrium defect concentrations, can be higher than that of common energy storage technologies such as lithium batteries and supercapacitors. We discuss storage of solar energy and electrical energy (through ion bombardment) using defects.

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