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Quantum Monte Carlo calculations of defects in aluminum[1] RANDOLPH Q. HOOD, Lawrence Livermore National Laboratory, PAUL R.C. KENT, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — We use first-principles fixed-node diffusion quantum Monte Carlo to calculate the energetics of point defects in bulk FCC aluminum demonstrating a very high accuracy when compared to experiment. Aluminum has been well studied experimentally as a "simple" metal prototype for investigating the effects of radiation damage such as void formation and helium embrittlement. Often accuracies at the level of milli-electronvolts are required, which is not achieved even for the simple case of pairs of vacancies in aluminum, using common density functionals. Perhaps surprisingly, even single vacancy energies are not reliable in many simple structural materials. Also presented are results for the bulk properties of aluminum - the equilibrium lattice constant, the cohesive energy, and the bulk modulus. These calculations bring a new level of rigor to the study of defects in metals.

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