Abstract Submitted
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**Calculating self diffusion in Mo using the AM05 density functional** THOMAS R. MATTSSON, Sandia National Laboratories, NILS SANDBERG, Royal Institute of Technology, RICKARD ARMIENTO, University of Bayreuth, ANN E. MATTSSON, Sandia National Laboratories — Vacancy diffusion is a major mechanism of mass transport in solids. While the motion of vacancies and interstitials is largely understood for fcc metals like aluminum [1], important questions remain for bcc metals. We present first principles and model potential simulations of self-diffusion in Mo, compare the results to available experimental data, and discuss the magnitude and origin of different contributions to the diffusion. The density functional AM05 [2] is employed to calculate formation energies and diffusion barrier for vacancy migration. AM05 has been successfully applied to a wide range of different solids [3] and is shown to perform well also for Mo. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. [1] N. Sandberg, B. Magyari-Kope, and T.R. Mattsson, PRL 89, 065901 (2002). [2] R. Armiento and A. E. Mattsson, PRB 72, 085108 (2005). [3] A.E. Mattsson, et al. JCP 128, 084714 (2008).

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