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Theoretical stability of Eu dopant in diamond WENHAO HU, MICHAEL E. FLATTÉ, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa — Due to their extremely long spin coherence times, rare earth ions are promising candidates for high resolution magnetic sensing. In addition, recent progress on high resolution magnetometry based on the diamond NV center suggests that the combination of diamond and rare earth ions might have perform well. In this article, we simulated europium complexes in diamond using density functional theory in the LSDA+U approximation. We used a 64-atom supercell for the diamond host, inserted Eu and removed 1-4 carbon atoms; atomic positions were allowed to relax with a force precision of 1.0 mRy/a.u. The formation energies of possible configurations of charged Eu in diamond were investigated. The first order Markov-Payne correction was used to remove the effects of the supercell size and fictitious charge background. The formation energy for substitutional Eu is very large, originating from the limited relaxation space for the nearest neighbor carbons, however the formation energy is much lower with 1-3 surrounding carbon vacancies. We find the most stable configuration is the +1 charged Eu with 1 neighboring vacancy. The work was supported by an AFOSR MURI.

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