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Bistable lattice position of a single magnetic dopant in a semiconductor JEFFREY M. MOORE, VICTORIA R. KORTAN, CÜNEYT ŞAHIN, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa, JUANITA BOCQUEL, PAUL M. KOENRAAD, Department of Applied Physics, Eindhoven University of Technology, MICHAEL E. FLATTÉ, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa — Electronic control of the lattice position of individual dopants has been demonstrated recently, including displacement of a single Si dopant in the surface layer of GaAs by a scanning tunneling microscope (STM)[1]. Fe dopants in GaAs have internal spin degrees of freedom associated with their core d states which can also be manipulated using a STM[2]. A reversible and hysteretic change in the topography measured near a single Fe dopant is observed when a negative bias voltage is applied. To determine if a lattice displacement is responsible, we have performed first-principles calculations to evaluate the formation energy of a single Fe atom embedded in GaAs as a function of displacement from the substitutional site. Our calculations support the existence of a second stable configuration, characterized by a displacement accompanied by a change in atomic configuration symmetry about the Fe from four-fold to six-fold symmetry. These results expand the range of demonstrated local configurational changes induced electronically for dopants, and thus may be of use for sensitive control of spin-spin interactions between dopants.

[1] J. K. Garleff et al., Physical Review B 84, 075459 (2011).

[2] J. Bocquel et al., Physical Review B 87, 075421 (2013).

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