Abstract Submitted
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The effects of adsorbates on surface morphologies and energies of iron-gallium alloys[1] HUI WANG, Department of Physics and Astronomy, University of California, Irvine, ALISON FLATAU, Department of Aerospace Engineering,University of Maryland, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Materials with large magnetostriction are extensively used in sensors, actuators, micro electromechanical systems, and energy-harvesters. Fe-Ga alloys (Galfenol) are very promising rare-earth free magnetostrictive materials. Investigation on surface energies of Galfenol based on density functional calculations (DFT) may provide fundamental understandings and guidance to further optimize the performance of Galfenol. Our DFT calculations predict that Ga-covered (110) surface of Galfenol is more stable in Ga-rich condition, while Ga-covered (001) surface become more favorable in Ga-poor condition, consistent with experimental observations. Moreover, we also study the environmental effects on surface energies of Galfenol and find that chemically adsorbed atoms (e.g. oxygen atoms) may change the surface energies, pointing out a feasible way of tuning the surface orientation of Galfenol to maximize its magnetostriction for practical application.

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