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Ab-initio study of the electron-phonon interaction of a single Fe adatom on the MgO/Ag(100) surface

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Controlling the magnetic moment of individual atoms is a technologically important challenge, with applications as high density storage devices. Breakthrough experimental studies have recently shown that it is possible to create stable magnetic quantum states in individual adatoms [1–3]. While the role of electronic interactions on the magnetic stability has been thoroughly investigated theoretically [4–6], the coupling with phonons has attracted much less attention. The aim of this work is to study, via ab-initio calculations, the effect of the electron-phonon interaction (EPI) in Fe adatoms deposited on MgO/Ag(100), a benchmark system where the EPI is believed to determine to large extent its magnetic stability [3]. Here we present the calculated electronic structure and vibrational dynamics of this system, including the local vibrations of the adatom. Furthermore, we analyze the effect of the EPI on the magnetic stability via the renormalization of the electronic properties of the adatom.

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Summary

Topic

1. Electrons and spins

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