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Ab initio study of Mg self-diffusion on Mg(0001) terraces and steps[1] MARAL AMINPOUR, MARISOL ALCANTARA ORTIGOZA, TALAT RAHMAN, Department of Physics, University of Central Florida, Orlando, 32816 — The high density of states (DOS) at the Fermi level and high density of quasi-free electrons result in a singular behavior for Mg surfaces and thin films. We find, however, that the DOS around the Fermi level, surface energy and cohesive energy converge beyond 15 layers. We also show that the Friedel charge density oscillations of Mg(0001) are more complex than depicted previously by 1D and 2D plots. These oscillations are, in fact, responsible for the stacking fault of Mg adatoms and islets on Mg(0001) and also, indirectly, for the low adatom self-diffusion barrier (20 meV) on Mg(0001), which is in agreement with effective-medium theory calculations. [1] We will compare this barrier with that of Mg adatom on a narrow terrace and across the steps on Mg(0001), as well as with predictions from Kinetic Monte Carlo simulations made to fit the growth mode observed for Mg/Mg-thin-films via scanning tunneling microscopy.

[1] Z.J. Tian, U. Yxklinten, B.I. Lundqvist and K.W. Jacobsen.Surf. Sci.**258** (1991), p. 427

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Maral Aminpour
Department of Physics, University of Central Florida, Orlando, 32816

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