**A First Principles Study of Stacking Fault and Surface Energies in Magnesium**

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Stacking fault and surface energies have been calculated for the basal and prismatic plane in magnesium using the first-principles ABINIT code. [1]

In extension of work by Uesugi et al. [2] calculations are presented for intrinsic, extrinsic and twinned stacking fault structures using the supercell approach [3]. Accordingly the generalized stacking fault energy is determined which represents the energy variation as a function of displacement of the crystal fault.

In order to achieve appropriate convergence of the energy calculations it is necessary to calibrate by determining the surface properties e.g. the surface energy, work function etc. [4]. In particular, the present work shows how careful choice of computational parameters avoids the usage of the somewhat spurious, in the present case, surface dipole correction.

[1] Gonze X., et al., *Comput. Mat. Sci*., 2002, **25**, 478-492. (The ABINIT code is a common project of the Université Catholique de Louvain, Corning Incorporated, and other contributors. See http://www.abinit.org.) [2] Uesugi T., Kohyama M., Kohzu M., Higashi K., *Mat. Sci. Forum*, 2003, **419-422**, 225-230. [3] Chetty N., Weinert M., *Phys. Rev. B*, 1997, **56**, 10844-10850. [4] Wachowicz E., Kiejna A., *J. Phys.: Condens. Matter*, 2001, **13**, 10767-10776.

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