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Phase diagram for the Ni/Al_2O_3 interface and relationships to adhesion XIAO-GANG WANG, JOHN SMITH, Delphi Research Labs, Shelby Township, Michigan 48315, USA — First-principlescalculations conducted over a broad range of atomic configurations havebeen used to determine the phase diagram and work ofseparation for Ni/Al_2O_3 interfaces[1]. Seven interfacial phases have been identified.The results reveal that the strongest (O-rich) phases derive theirstrength from ionic Ni-O bonds across the interface, reminiscent ofNiO. The Al-rich phases are also strong, exhibiting a mixof Ni_3Al-like and Al_2O_3-like interfacial bonds. The stoichiometric interfaces arethe weakest since they are formed from the ground-state Al_2O_3(0001)surface. [1] X.-G. Wang, J. Smith, A. G. Evans, Phys. Rev. B 74, 081403(2006).

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