

Abstract Submitted  
for the MAR05 Meeting of  
The American Physical Society

**Ab Initio Hartree-Fock Calculation of Electronic Band Structure in Transition Metal Silicides** ALVARO POSADA-AMARILLAS, Dept de Investigación en Física, JOSÉ SAMANIEGO-REYNA, Centro de Ciencias de la Materia Condensada, UNAM-Ensenada, MARGARITA FRANCO-ORTIZ, Programa de Posgrado en Ciencias (Física), DCEN, Universidad de Sonora, DONALD GALVÁN, Centro de Ciencias de la Materia Condensada, UNAM- Ensenada — *Ab initio* Hartree-Fock method has been used to calculate electronic properties in  $\text{CoSi}_2$  and  $\text{NiSi}_2$ . *A posteriori* DFT energy correction has been included in order to test the effect of electronic correlation using B3LYP, VWM and LDA approximations for the correlation term. No correlation and VWM correlation results are compared, finding that the electronic correlation produces band gaps at specific high symmetry points in the first Brillouin zone. Total energy results indicate that correlation energy is high compared to the Hartree-Fock energy for both Co and Ni silicides. This is an indication that  $\text{CoSi}_2$  and  $\text{NiSi}_2$  are highly correlated systems.

Alvaro Posada-Amarillas  
Dept de Investigación en Física

Date submitted: 23 Nov 2004

Electronic form version 1.4