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2 PdpSc *

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1 Q.341 L12 — — DO 22 . 1 o.eel- X=Sc

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100—

Ti V Cr Mn Fe Co Ni CU

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2 -Pd3Co *

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rromagnetic
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8.0 8.5 9.0 9.5 1 0.0 Number of Valence Electrons/Atom

10.5

0
2 -Pd C

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1 o.e21

I I

I I I I I I

p
-8 -6

I I I

-4 -2 0 2 4 -8 -6 -4 -2

Energy (eV)

0 2 4

FIG. 2. LDA calculated NM total DOS for Pd3X in the L12

and DOq2 structures. The insets denote N(EF). An asterisk
denotes the more stable structure predicted by total energy
calculations in the absence of magnetic ordering. Note that
the more stable structure has a lower N(EF)

nonmagnetically predicted D022 structure. Thus, while

the correlation between the calculated quantities N(EF)
vs E(Llz) —E(DOzz) holds, it leads to incorrect predic-tions for the stability of Pd3Cr, Pd3Mn, and Pd3Fe. The
generalized perturbation method calculations [4], based on

similar DOS arguments [diamond symbols in Fig. 3(a)]
likewise predict Pd3Cr, PdsMn, and Pd3Fe (and even

Pd3Sc and Pd3Ti) to be stable in the DOzz structures, in conllict with experiment [2].

In this paper we explain this puzzle by noting that,

while a large N(EF) indeed implies a destabilizing factor
for the one-electron ("band") energy, it also leads (in

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TABLE I. LDA calculated total energy difference (in meV/atom) BE = E(Llz) —E(DOzz) and the ferromagnetic (FM) DOS
at Fermi energy N(EF) (in states/eV spin) for the Llz and DOzz structure nNMj ET BT /Xi2 9.93 Tf 350.22 782.56 Td (for)TjNotT BT /Xi2 7.96 Tf 741.33 7

7

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Pd3Cr
Pd3Co
Pd3Ni
Pt3Cr
Pt3Co

b,H(L12)
NM

126
155

61 —68
31

FM

—9
64

43 —185 —42

51
160

62 —139
42

AH(DOpg)
FM

11
49

44 —161 —26

TABLE II. Nonmagnetic (NM) and ferromagnetic (FM) for-mation enthalpies, hH [in meV/atom, Eq. (1)], of some com-pounds. AH's are taken with respect to the NM fcc Pd, Pt, FM fcc Ni, FM fcc Co, and anti-FM bcc Cr, respectively.

We thank Professor Alan