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Chemical trends in ground- and excited-state properties of
interstitial 3d impurities in silicon
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A spin-polarized local-density Green interstitial
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TABLE I. Calculated (Refs. 8 and 9) and observed (Refs. 1 and
11) g values and hyperfine coupling constants A of interstitial 3d im-
purities in Si. Asterisks denote calculated values of contact interac-
tion alone.. A is in unit of 10 4

crn ~. Error bars (Ref. 11) are
given only in the case of Si:Ti+ [g = 1.99806 +0.000 04,
A

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Energy of Interstitial Si:3d
Calculation (Unrelaxed)
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