AB INITIO STUDY OF THE LOWEST ENERGY STATES OF CUSI USING MULTICONFIGURATION VALENCE BOND METHOD

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An all electron *ab-initio* multiconfiguration valence bond method is applied to study the lowest energy states of CuSi. This detailed gas phase study of copper-silicon molecule should allow us to better understand the bonding occuring at the copper-silicon interface in bulk material used in the construction of electronic devices.

The molecular basis consists of Hartree-Fock wavefunctions and includes occupied and unoccupied virtual orbitals for both Cu and Si atoms. By increasing the number of excited virtual states in the basis set we have converged the electronic energies of the first $^2\Sigma$, $^2\Pi$, $^4\Sigma$, and $^4\Pi$ states. These results are used to determine the spectroscopic molecular constants of CuSi.