# Magnetite electronic structure from multi-configurational ab-initio calculation

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Magnetite's structure ($Fe_3O_4$) has been known since 1915 [1]. It is assumed to form an inverse spinel structure which is usually represented as $B^{III}(A^{II}B^{III})O_4$. Trivalent iron ions completely occupy the tetrahedral sites, while the octahedral sites are randomly populated by both trivalent and divalent ions. In our study, we have examined one of the possible configurations for the distribution of these multivalent ions. In this work ground state energy is calculated for different spin multiplicity available for a given size cluster. It is shown that there exists an optimal high spin multiplicity for which the electronic energy of the system is the lowest. Excited state calculations show a very dense state population, resulting in a narrow band gap close to the experimental result.

The problem of valency and oxidation state of an atom in a crystal is discussed in context of quantum chemical calculations [2] of bulk $Fe_3O_4$ in embedded cluster approach. Results of the calculations for high spin ground state support experimental valency. We employed the MOLCAS software package [3] for our calculations, particularly the recent implementation of the SCEPIC (Self-Consistent Embedded Potential for Ionic Calculation) program [4].

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