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Elastic and Electronic Properties of some Fe compounds

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A new stress-strain method is employed to study the elastic properties of simple elements including the recently proposed anti-ferromagnetic phase of hcp epsilon-Fe. The results are compared with the conventional energy-strain method. At low pressure, results on epsilon-Fe show a slight improvement with experimental elastic constants and phonon density of states but serious discrepancy still persist at high pressure. We also examined electron correlaton effects on the electronic spectra of Fe containing minerals with the LDA+U model. We calculated the photoelectron spectra of several Fe containing minerals and examine the recently reported spin transition in ferropericlases. It is found that local environment of the Fe impurities plays an important role on the spin transition pressure and the ground electronic state. The super-exchange interactions between Fe2+ along the Fe-O-Fe chains led to an anti-ferromagnetic ground states. The predicted spin transition pressures are found to increase with the Fe content.