Electronic structure and magnetic properties of LaFeAsO- and FeSe-based superconductors

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Ab initio calculations of the volume dependent band structure and the exchange enhanced paramagnetic susceptibility were performed for LaFeAsO and FeSe-based systems within the local spin density approximation. It is found that these systems are close to magnetic instability with dominating enhanced spin paramagnetism, and the van Hove singularities are revealed in the electronic spectra. The calculated values of the density of states at the Fermi level and paramagnetic susceptibility exhibit a strong dependence on the structural parameters, such as unit cell volume V and especially the height Z of pnictogen/chalcogen species from the Fe plane. The puzzling experimentally observed pressure effects on susceptibility and superconductivity in LaFeAsO and FeSe-based systems are explained in terms of the pressure dependence of structural parameters V and Z.