

## ELECTRONIC STRUCTURE AND PROPERTIES OF NOVEL LAYERED SUPERCONDUCTORS

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### S u m m a r y

The electronic energy structures and magnetic properties of layered superconductors  $RNi_2B_2C$ ,  $RFe_4Al_8$ , and FeSe are systematically studied, by using the density functional theory (DFT). The calculations allowed us to reveal a number of features of the electronic structure, which can cause the manifestation of peculiar structural, magnetic and superconducting properties of these systems. It is demonstrated that the Fermi energy  $E_F$  is located close to the pronounced peaks of the electronic density of states (DOS). The main contribution to DOS at the Fermi level arises from  $3d$ -electrons. The calculations of the pressure-dependent electronic structure and the magnetic susceptibility in the normal state indicate that the novel superconductors are very close to a magnetic instability with dominating spin paramagnetism. It is shown that experimental data on the pressure dependence of the superconducting transition temperature in FeSe correlate qualitatively with the calculated behavior of DOS at  $E_F$  as a function of the pressure.