

POZVÁNKA

na seminář oddělení 15 Fyzikálního ústavu AV ČR, v.v.i.

Seminář se koná

v pondělí 1. prosince 2014 v 10:00

v zasedací místnosti budovy B
Fyzikálního ústavu AV ČR, Cukrovarnická 10, Praha 6.

Na programu je přednáška

Ab initio study of piezomagnetic effect in Mn-antiperovskites

kterou prosloví

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Abstrakt

The magnetocaloric and magnetoelastic coupling that often occur together in magnetically frustrated materials have a great potential for practical applications ranging from magnetic refrigeration to data processing and storage. Negative thermal expansion (NTE) close to the Néel temperature and a large magnetovolume effect have been measured recently in Mn_3NiN using temperature dependent neutron powder diffraction [J. Appl. Phys. 114, 123902 (2013)]. This theoretical work comprises a comparative study of the piezomagnetic effect in three closely related related Mn_3XN ($X = \text{Ni}, \text{Sn}, \text{In}$) antiperovskites, based on the foundations of a recent DFT model [Phys. Rev. B 88, 024417 (2013)] of anisotropic thermal expansions and large magnetoelastic coupling. It relies on the framework of the projector augmented-wave (PAW) method as implemented in the VASP code.