## POZVÁNKA

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

### Seminář se koná

### ve čtvrtek 20.2. 2020 ve 14:00

v zasedací místnosti budovy A (vedle knihovny) Fyzikálního ústavu, Cukrovarnická 10, Praha 6.

Na programu je přednáška

# The insight into the Dzyaloshinskii-Moriya interaction through first-principles study of chiral magnetic structures

kterou prosloví

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#### Abstrakt

The purpose of the work is to gain deeper insight into microscopic formation of the Dzyaloshinckii-Moriya interaction (DMI). The work aims at the development of the physical picture able to address apparently contradicting conclusions of recent studies concerning the location of the DMI energy in the real and reciprocal spaces as well as the relation between values of the atomic moments and the DMI strength. The main tool of our study is the first-principles calculations of the energies of the spiral magnetic states with opposite chiralities. We suggest a new method of the calculation of the spiral structures with account for the spin- orbit coupling (SOC). It is based on the application of the generalized Bloch theorem and generalized Bloch functions and allows to reduce the consideration of arbitrary incommensurate spiral to small chemical unit cell. The concrete calculations are performed for the Co/Pt bilayer. We consider the distribution of the DMI energy in both real and reciprocal spaces and the dependence of the DMI on the number of electrons. The results of the calculations reveal a number of energy compensations in the formation of the DMI. The physical process of the DMI formation is connected with the difference in the hybridization of the Co and Pt states for  $\mathbf{q}$  and  $-\mathbf{q}$  spirals under the influence of the SOC and broken spatial inversion. The application of the new method to the calculation of the magnon energies in systems with DMI is briefly addressed.