

Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensed Matter Physics
of Charles University has a pleasure to invite you to attend the seminar

on 15 November 2018 at 13:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Seminar room F052



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Searching for the rare-earth free permanent magnets with structure predicting methods: possibilities and limitations

Structure prediction based on evolutionary/genetic algorithm methods combined with density functional theory calculations provides material scientists with a tool to predict from scratch the stable structure of a compound just with the mere knowledge of its composition. In practice, however, the process of accurate prediction of a new structure by simulations may be as time consuming as obtaining it in the lab. Here I will present some result of searching for new rare-earth free magnetic structures within the Horizon 2020 project NOVAMAG by using the evolutionary code USPEX and ab-initio code VASP. Based on this experience, I will bring into discussion the limitations as well as the possibilities for making the best use of structure predicting methods.

