Computer calculations of electronic properties of selected solid state materials: permanent magnets, hydrogen storage materials or magnetocalorics

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Short general introduction:

Quantum mechanical atomic models allowed in the twenties to explain a number of properties of all single element in the periodic table. The natural next step in the development of this theoretical model was to go from a single atom to a diatomic molecule etc. The culmination of this journey are models of solids containing in the one system many atoms of various types. An example might be a model of commonly known neodymium magnet with formula $Nd_2Fe_{14}B$ in which the only parameters are the atomic numbers Z of the individual elements. 3D geometry of the system can be based on the X-ray crystallographic structure, or determined fully theoretically. The numerical solution of the equations for all the electrons interacting in the system determines the band structure of the studied material, and hence a number of macroscopic properties, such as modulus of elasticity or magnetization.

Department of Solid State Theory (Z2) uses for the calculations a supercomputer with a dedicated architecture (http://www.ifmpan.poznan.pl/en/scientific-divisions/department-of-solid-state-theory-equipment.html) together with a wide range of specialized software based on the Linux operating system.

Suggested research subjects are three classes of materials (optional):

1) magnetic materials containing heavy elements;
2) materials for hydrogen storage and
3) magnetocalorics - materials for magnetic refrigerators.

The three above-mentioned topics, arousing keen interest in the global scientific community, are now extensively studied by our team in close collaboration with a number of experimental groups from the country and the world.

Research project objectives and methodologies:

Objectives of the study will depend upon the classes of materials.

1) For magnetic materials containing heavy elements the main purpose will be to increase the magnetocrystalline anisotropy of the compounds by structural modifications - doping.
2) For hydrogen storage materials the goal will be to find the stable compounds with the greatest hydrogen storage potential, to determine their electronic properties and to find specific dopants which improve their stability.
3) For magnetocalorics the objective is to increase the critical cooling power parameter RCP of YCo_2 alloys modified with chemical and topological disorder.

In every case, the band structure ab-initio calculations will be used as the main method.