

SEMINARIUM Z MAGNETYZMU I NADPRZEWODNICTWA

Uprzejmie zawiadamiamy, że w **ŚRODĘ**

10 grudnia 2014 r., o godz. 10:00

w sali D (bud. 1) odbędzie się seminarium, na którym

Dr Giovanni Pizzi

École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

wyłosi referat na temat:

The high-throughput infrastructure AiiDA and the study of local polarization in perovskites

"Materials by design" is a new and extremely powerful approach In Materials Science, where rather than choosing one material and calculating its properties, one identifies instead a desired property and looks for the best material that optimizes it. This approach requires though to build large databases of computed properties of materials. A key challenge becomes therefore the need of a "materials' informatics" infrastructure to automatically prepare, execute and monitor workflows of calculations for large classes of materials, and then retrieve and store the results in a format that is easily browseable and queryable. To this aim, we are developing an open-source platform for high-throughput (AiiDA: "automatem Interactive Infrastructure and Database for Atomistic simulations", www.aiida.net), that uses an advanced storing scheme to allow for highly flexible queries, combined with a REST API that exposes in a standard format the data stored in the database for further programmatic access. After describing the infrastructure, I will show some examples of application, focusing in particular on the study of the local polarization in perovskites. Many of these systems display a high-temperature paraelectric cubic phase (with zero net polarization), whose microscopic nature is still debated. Indeed, by performing a systematic study of a selected class of these systems, we are able to identify different behaviors, and in some materials like BaTiO₃ and KNbO₃ we find the emergence of local ferroelectric dipoles even in the paraelectric phase.

Serdecznie zapraszamy

Roman Puźniak
Henryk Szymczak
Andrzej Wiśniewski