# Fall 2016 Joint Colloquium
# Materials Department & Materials Research Laboratory

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Center for Physical Sciences and Technology
Vilnius, Lithuania

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11:00 am, ESB 1001

**Defects in solids: agents of broken symmetry**

In pristine semiconductors and insulators many electronic transitions are either forbidden or very weak because of selection rules imposed by the high symmetry of the solid. In many ways point defects (impurities, vacancies, interstitials, and various complexes) can be thought of systems with broken symmetry where formerly forbidden transitions become allowed. Depending on the application of the material, these new transitions can be either beneficial, neutral, or detrimental. The example of beneficial properties are defects that are currently investigated in view of their application in quantum information processing and nano-metrology. The example of detrimental properties are defects that serve as nonradiative recombination centers in optoelectronic devices. In both cases, defects affect the properties of materials dramatically.

Over the past decade computational techniques to study defects in solids have finally reached the level where a direct comparison with experiment can be made. Moreover, these techniques can provide the microscopic understanding that can complement and guide the experimental work. In this talk an overview of some of the author's recent work on the electronic structure of point defects will be given. In the beneficial domain (defects for quantum information processing and nano-metrology), electron-phonon coupling in nitrogen-vacancy and silicon-vacancy centers in diamond will be discussed. In the detrimental domain, nonradiative transitions at defects in group-III nitrides will be analysed and the implications of these findings for efficiencies of nitride light-emitting diodes will be highlighted.

**Bio**

Audrius Alkauskas studied physics in Vilnius University (Lithuania). In 2006 he obtained a PhD degree in theoretical physics from the University of Basel (Switzerland). In 2006-2010 he was a post-doctoral fellow at Ecole Polytechnique Federale de Lausanne (EPFL). In 2011-2014 he was a post-doctoral fellow in the University of California Santa Barbara, working in the group of prof. C. G. Van de Walle. In 2014 A. Alkauskas joined the Center for Physical Sciences and Technology (FTMC) in Vilnius, Lithuania, becoming a Principal researcher in 2016. He leads the electronic structure theory group at FTMC. He is also holds a position of a visiting professor in Kaunas University of Technology in Kaunas, Lithuania. Scientific research interests of A. Alkauskas include the theory of radiative and nonradiative transitions in solids, as well as the theory of point defects for quantum information processing.

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Hosted by Chris Van de Walle.