# 凝聚态物理前沿论坛

## 第五十一讲

**题　　目：Calculating defects and surfaces in diamond and $TiO_2$**

**报 告 人：Prof. Peter Deák,**
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**时　　间：2017年8月30日 (周三) 上午 09：00**

**地　　点：固体所3号楼221会议室**

## 报告摘要：

Defects and surfaces modify the electronic and optical properties of non-metallic solids, so these effects have to be known and taken into account in materials engineering. Since both the bulk and the surface contain many defects, disentangling the consequences requires the help of quantum mechanical model calculations. Theoretical defect physics, using the standard local or semi-local approximations of density functional theory, has been quite successful in traditional semiconductors, however, wide band gap materials are a serious challenge. In this talk I show first, how screened hybrid functionals can be used to overcome earlier problems, leading to an unprecented accuracy. I will then consider two examples: the single photon emitter NV(-) center in diamond and photocatalytic water splitting by $TiO_2$.

## 报告人简介：

Peter Deák, Professor of Physics at the University of Bremen and Head of the Electronic Materials Group at the Bremen Center for Computational Materials Science, has received his PhD in Physics from the University of Budapest (Hungary) in 1984. After postdoc years at the SUNY/Albany (US), at the MPI Stuttgart and at the U. Kaiserlautern (Germany), he obtained the title, Doctor of the Hungarian Academy of Science, in 1994 and has become Professor of Surface Physics and Head of the Applied Surface Science Laboratory at the Budapest Institute of Technology and Economics. Since 2003 he lives in Germany. His expertise is in the atomic scale quantum mechanical simulation of electronic materials (especially defects and surfaces), and in the materials science and technology of electronic and electric devices, functional coatings, plasma discharges, low-pressure synthesis of diamond, and of photocatalysis. He is the author of about 200 publications and editor of 3 books. He is the member of the editorial board of Physica Status Solidi.