**报告题目:** Hybrid inorganic/organic interfaces from a semiconductor's perspective

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**地点**：理科楼郑裕彤讲堂

**摘要：**

Hybrid inorganic/organic systems have opened up new opportunities for the development of (opto)electronic and photovoltaic devices due to their potential of achieving synergy by combining the best features of two distinct material classes. With view to optoelectronic applications, ZnO is currently being investigated as the inorganic component. However, the rich phase diagram of the common polar ZnO surfaces [1] makes the growth, characterization and the theoretical description of the organic/ZnO interface a challenge task.

Here we use density-functional theory in combination with *ab initio* thermodynamics [2] to develop an atomistic understanding of the ZnO surface phase diagram and organic/ZnO interfaces. In this approach externally controlled factors like temperature or partial pressures are introduced through the atomic chemical potentials. However, the role of the electron chemical potential (or Fermi level) for surfaces has so far been ignored. For the O-polar (000-1) surface I will demonstrate that electrons (holes) from bulk donor (acceptors) can stabilize hitherto overlooked structures that do not fulfill the electron counting rule, which usually results in no net surface charge and in a semiconducting surface. For prototypical adsorbates like pyridine [3] or 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquino-dimethane (F4TCNQ), I will discuss our model for the interface structure and elucidate the role of the ZnO Fermi level on the level alignment at these hybrid interfaces. I will also address the limitations of common density functionals and show how they can be overcome by using exact-exchange based functionals or quasiparticle energy calculations [4].

\* This work was performed in collaboration with Y. Xu, O. Hofmann, N. Moll, B. Bieniek, C. Freysoldt and M. Scheffler.

References

[1] C. Wöll, Prog. Surf. Sci. 82, **55** (2007).

[2] K. Reuter and M. Scheffler, Phys. Rev. B **65**, 035406 (2001).

[3] O. T. Hofmann, J.-C. Deinert, Y. Xu, P. Rinke, J. Stähler, M. Wolf,   
 and M. Scheffler, submitted to Advanced Materials

[4] C. Freysoldt, P. Rinke, and M. Scheffler, Phys. Rev. Lett. **103**, 056803 (2009)