Gemeinsames Kolloquium
der Sonderforschungsbereiche 445, 491 und 616

Vortragender: **Dr. R. I. Eglitis**

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Gast von Prof. Entel

Thema: ***Ab initio* calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces as well as Nb impurity segregation towards the $SrTiO_3$ surface**

Abstract: While the (001) surfaces of ABO_3 perovskites, such as $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $SrZrO_3$, $PbZrO_3$ and $BaZrO_3$ have been extensively studied [1-5], much less is known about the (011) surfaces. On the (001) surfaces, I consider both AO (A=Sr, Ba, Pb or Ca) and BO_2 (B=Ti or Zr) terminations. The (001) surface AO layer is found to relax inward for all seven materials with the sole exception of SrO-terminated $SrTiO_3$ (001) surface first layer O atom.

My calculated surface rumplings of 6.77 % for the SrO-terminated $SrZrO_3$ (001) and 3.32 % for the PbO-terminated $PbZrO_3$ (001) surfaces are almost ten times larger than those of the corresponding ZrO_2-terminated $SrZrO_3$ and $PbZrO_3$ (001) surfaces [5].

As for the (011) surfaces, I consider three types of surfaces, terminating on a BO layer, A layer and O layer. Turning now to the surface energies, I find that both the AO and BO_2-terminated (001) surfaces are about equally energetically favorable and may co-exist. In contrast, I see very large differences in the surface energies on the ABO_3 (011) surfaces. I demonstrate that Nb is a shallow donor in $SrTiO_3$ and discuss also its segregation towards the $SrTiO_3$ surface [6].

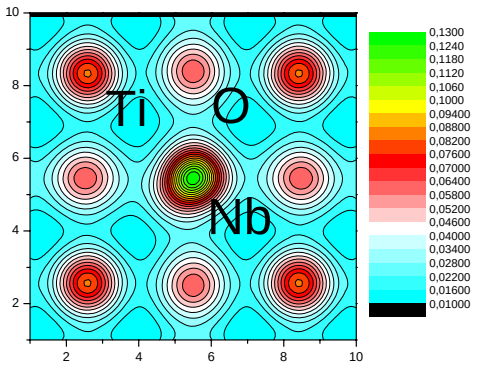

Fig. 1 Total charge density map for Nb doped $SrTiO_3$ calculated by means of hybrid B3PW method.

References
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3. R. I. Eglitis and D. Vanderbilt, Phys. Rev. B **77**, 195408 (2008).
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Zeit: ***Dienstag*, 12. Juli 2011, 12:00 Uhr** (Sondertermin)

Ort: Gebäude **MD, Raum 349** (Campus Duisburg)
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Interessenten sind herzlich willkommen

Prof. Dr. A. Lorke	Prof. Dr. Dr. h. c. H. Zabel	Prof. Dr. M. Horn-von Hoegen
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