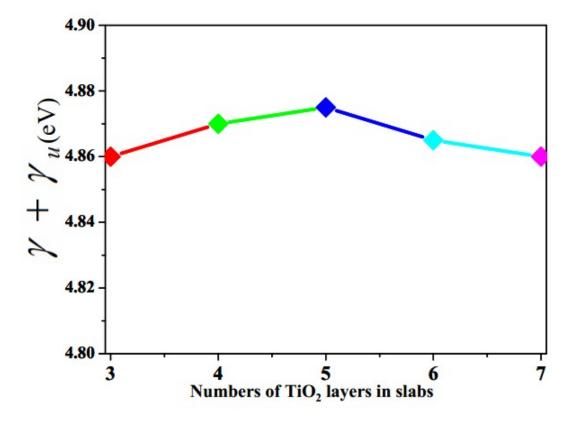
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2016

Unexpectedly rich structures of rutile $TiO_2(011)$ -(2×1) and driving forces behind their formations: an *ab initio* evolutionary study

Qinggao Wang^{1,31}, Artem R. Oganov^{2,1,4,5}, Oleg D. Feya¹, Qiang Zhu⁴, and Dongwei Ma³

- 1 Moscow Institute of Physics and Technology, 9 Institutskiy Lane, Dolgoprudny City, Moscow Region, 141700, Russia
- 2 Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, 3 Nobel St., Moscow 143026, Russia
- 3 Department of Physics and Electrical Engineering, Anyang Normal University, Anyang, Henan Province, 455000, the People's Republic of China
- 4 Department of Geosciences and Center for Materials by Design, Stony Brook University, Stony Brook, New York 11794, USA
- 5 School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, Shanxi 710072, People's Republic of China



The changes of surface energy for unreconstructed TiO₂ rutile (011) with slab thickness

¹Corresponding author: wangqinggao1984@126.com