

# ***AB INITIO* SIMULATIONS ON PERFECT AND DEFECTIVE INORGANIC NANOTUBES AND NANOWIRES**

Yuri F. Zhukovskii<sup>1</sup> and Sergey Piskunov<sup>1,2,3</sup>

<sup>1</sup>Institute of Solid State Physics, University of Latvia, Latvia

<sup>2</sup>Faculty of Physics and Mathematics, University of Latvia, Latvia

<sup>3</sup>Faculty of Computing, University of Latvia, 19 Raina Blvd., Riga LV-1586, Latvia

e-mail: quantzh@latnet.lv

Inorganic nanotubes (NTs) and nanowires (NWs) are technologically important 1D nanomaterials. We consider results of theoretical simulations on BN, TiO<sub>2</sub> and SrTiO<sub>3</sub> nanostructures [1-6]. For *ab initio* calculations on single-wall (SW) and double-wall (DW) boron nitride [1,2] and titania [1-3] nanotubes as well as on SW strontium titanate NTs [4], we have applied the formalism of line symmetry groups describing one-periodic (1D) nanostructures with rotohelical symmetry. The NW symmetry is defined by both the structure of the prototype bulk crystal and the direction of the one-dimensional crystallographic translation periodicity within the formalism of rod groups [5]. Variety of experimental conditions accompanying synthesis of 1D nanostructures can certainly promote the appearance of point defects: native vacancies or antisites as well as substitutional impurities. These and other types of irregularities may occur in inorganic nanostructures as a result of the growth process or intentionally induced to modify their properties (example of simulation on defective BN NTs was considered in Ref. [6]). Using hybrid exchange-correlation functional PBE0 within the density functional theory [7] we have performed large-scale calculations on perfect and defective 1D nanostructures enumerated above.

## References

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