

SCC-DFTB Study of Chrysotile Nanotube

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Lizardite and chrysotile are the most abundant minerals of the serpentine group and share the same chemical formula $Mg_3Si_2(OH)_2$. Lizardite has a flat-layered structure and chrysotile, the less abundant, occurs as cylindrically or spirally wrapped nanotubes (Fig.1)[1]. Recent studies indicate that chrysotile could be used as support for the immobilization of metalloporphyrins as well as adsorbent of ions and molecules[2]. Chrysotile has been the target for designing advanced materials with enhanced properties. In this work the self consistent charge – Density Functional Tight Binding (SCC-DFTB) method was used to study stability, electronic and mechanical properties of chrysotile. The Slater-Koster parameters for MgX ($X = Mg, Si, O, H$) have been calculated and the SCC-DFTB calculations compared with respect to the DFT calculations. The bond lengths and angles are in good agreement with DFT results, with an error around 0.05\AA and 3 degrees, respectively. Chrysotile nanotubes with different chiralities and sizes have been calculated and their stability compared with respect to the lizardite. The SCC-DFTB calculations were performed using the deMon-nano and DFTB+ codes.

Keywords: Clay Mineral, DFT, SCC-DFTB, electronic and mechanical properties.

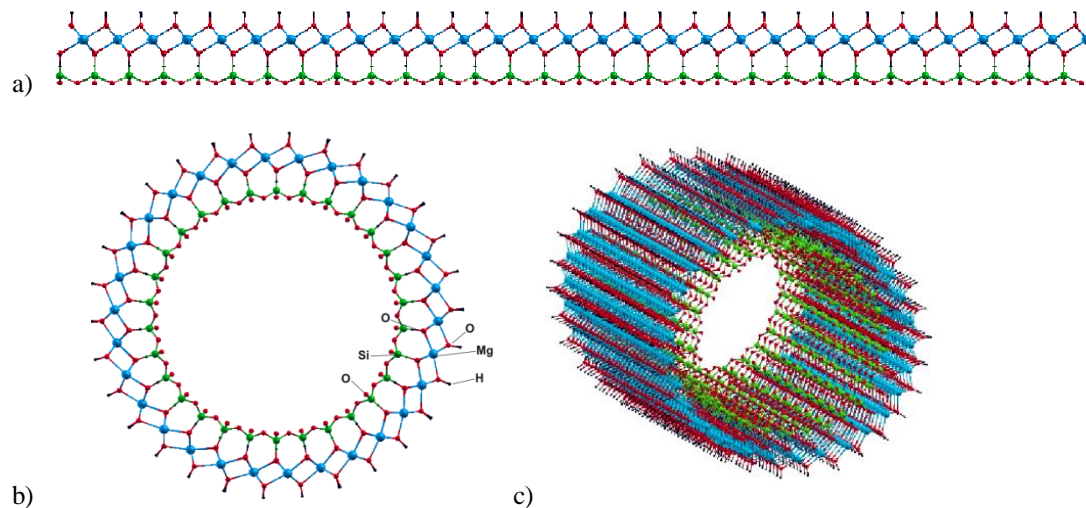


Figure 1. Structures of lizardite (2D) (a), chrysotile (2D) (b) and (3D) (c).

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[1] D. A. Philipe, Y. Yves, D. Raffaella, D. Roberto, J. Chem. Phys. **131**, 204701 (2009).

[2] S. Nakagaki, F. Wypych, J. Coll. Int. Sci., 315, 142 (2007).

[3] A. F. Oliveira, G. Seifert, T. Heine, H. A. Duarte, J. Braz. Chem. Soc. **20**, 1193 (2009).

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