A DFT study of (001) $CaSnO_3$ orthorhombic perovskite surface with adsorbed gases (NH_3 and CO)

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The $CaSnO_3$ (001) surface is here studied under the Density Functional Theory (DFT) framework with PBE and PBE0 functionals using Crystal14 program[1]. Two terminations of the pristine surface were studied, the first was surface terminated in CaO (CaO-**T**) that presented to be slightly more stable than the SnO_2 terminated, SnO_2-**T**. Carbon monoxide, CO, and ammonia and NH_3 gases were adsorbed over the SnO_2-**T** surface, said to be more reactive. The surfaces and adsorptions were evaluated using differential charge density maps, Density of States (DOS) and Raman intensities (through the Coupled-Perturbed-Hartree-Fock/Kohn-Sham algorithm). The CO adsorption was weaker than the NH_3 one. Both presented large shifts on the Raman spectra (Figs. 1 and 2), however only NH_3 presented a new intense Raman peak about 3098 cm^{-1}, this assigned to the stretch of the the hydrogen towards the superficial oxygen.The (001) of the $CaSnO_3$ perovskite presented sensor properties for the studied gases, and its interaction with NH_3 is noteworthy.

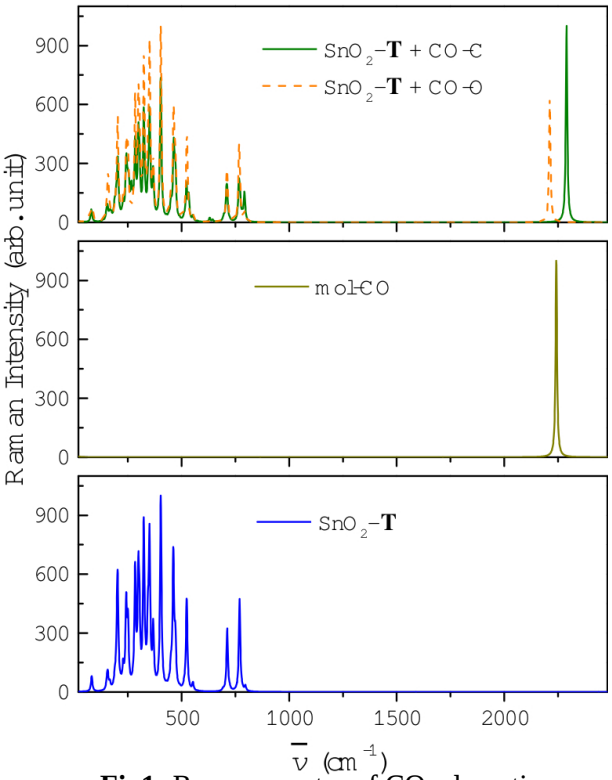

Fig1: Raman spectra of CO adsorption on SnO2 -**T** at PBE0 level

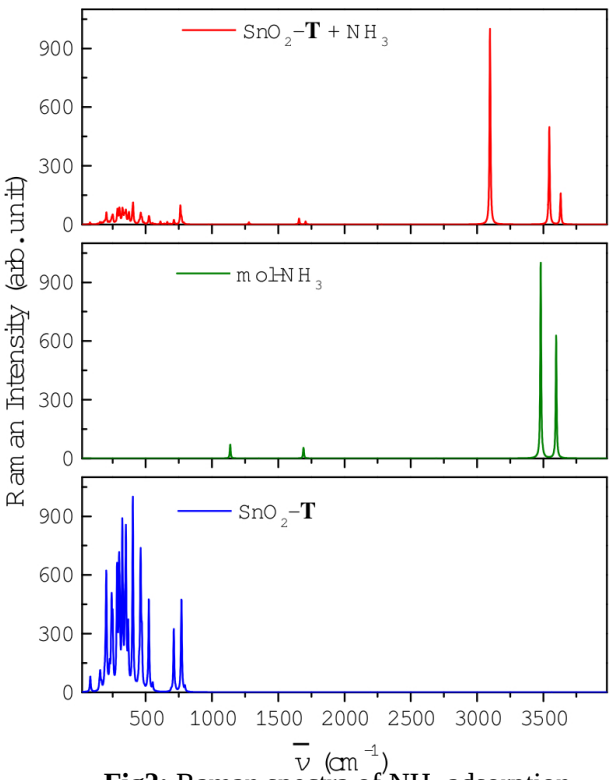

Fig2: Raman spectra of NH_3 adsorption on SnO2 -**T** at PBE0 level

References:

[1] R. Dovesi, V. R. Saunders, C. Roetti et al., CRYSTAL14 User's Manual (2014).