Ultra-thin a-Fe_2O_3: An *ab-initio* study

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Motivated by the recent synthesis of two-dimensional a-Fe_2O_3 [1], we use *ab-initio* calculations to investigate the structural, vibrational, magnetic, and electronic properties of single-layer (SL) and few-layer a-Fe_2O_3. For SL a-Fe_2O_3 (see Fig 1 (a)), the anti-ferromagnetic magnetic configuration is found to be the ground state. From the phonon band structure we conclude that SL a-Fe_2O_3 is dynamically stable. The calculated Raman spectrum reveals that the frequencies and Raman activities of the modes are significantly different from those of few-layers and bulk Fe_2O_3 which is shown in Fig 1(b). Temperature dependent magnetic properties are investigated using Monte-Carlo simulation with the calculated magnetic exchange parameters. It is predicted that the single layer structure exhibits magnetic phase transitions from a weak ferromagnetic to an anti-ferromagnetic state at T_C = 78 K. At room temperature, the average magnetization per Fe atom is found to be ~0.08 μ_B. The ground state is found to be a semiconductor with an indirect band gap of 0.75 eV and it exhibits a conductive and optically active mid-gap band originating from the outer Fe atoms. Furthermore, we investigate number of layer dependent electronic and vibrational properties of a-Fe_2O_3. The calculated dielectric functions for different thicknesses show that the prominent parts of the optical spectrum shift through the high energy when the thickness decreases, however, the peaks originating from the mid-gap states shift through the lower energy. More significantly, the calculated Raman spectra for different thicknesses reveal that few-layer structures exhibit a specific peak at ~660 cm^{-1} which does not appear for the bulk structure. Our findings are also consistent with the experiment results [1]. Its dynamical stability, weak magnetization at room temperature and semiconducting nature, single-layer a-Fe_2O_3 is a good candidate for nano-scale technological application.

Reference

[1] Balan *et al*. Nat. Nanotech. **13**, 602 (2018).

Figures

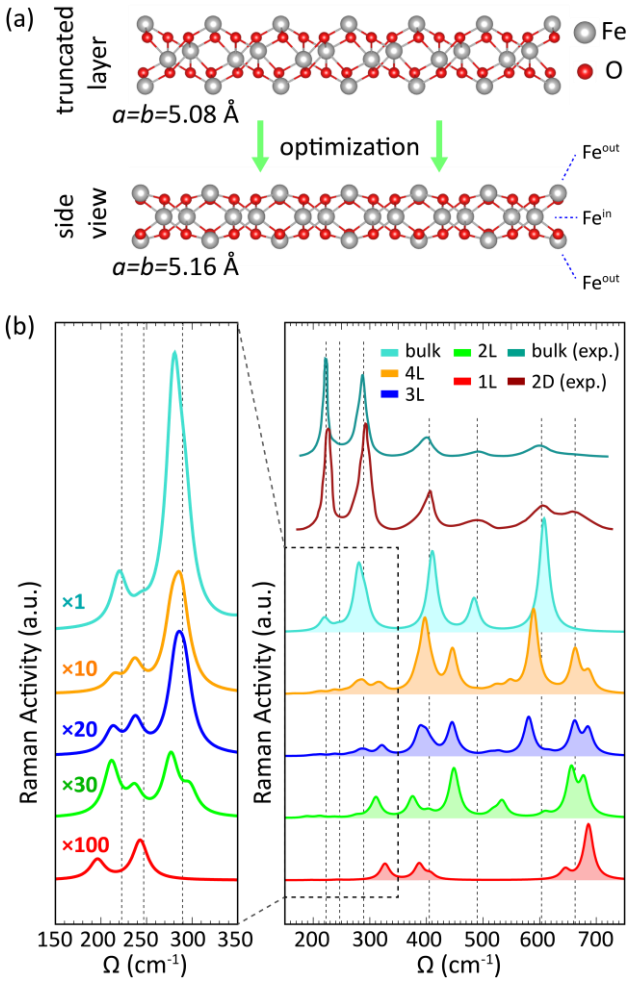

Figure 1: (a) Schematic representation of the optimization of SL a-Fe_2O_3 from the layer truncated from the bulk structure. (b) The calculated Raman spectra of SL, 2L, 3L, 4Land bulk structures. The right panel focuses in the peaks screened by the prominent peaks.