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First principles study of very thin TiO nanowires OGUZ GULSEREN, DENIZ CAKIR, Bilkent University — We have systematically investigated structural, electronic and magnetic properties of very thin TiO_x (x=1,2) nanowires as well as bulk-like (110) rutile nanowires by using the first principles plane wave pseudopotential calculations based on density functional theory. A large number of different possible structures have been searched via total energy calculations in order to find the ground state structures of these nanowires. Three dimensional structures are more energetic than planar ones for both of the stoichiometries (i.e. x=1,2). The stability of TiO_x nanowires enhances with its increasing radius, thus reaching sufficient coordination number of Ti and O atoms. All stoichiometric TiO_2 nanowires studied exhibit semiconducting behavior and have nonmagnetic ground state. There is a correlation between binding energy (E_b) and energy band gap (E_g) of TiO_2 nanowires. In general, E_b increases with increasing E_g. In TiO nanowires, both metallic and semiconductor nanowires are resulted. In this case, in addition to paramagnetic TiO nanowires, there are also ferromagnetic ones. We have also studied the structural and electronic properties of bulk-like rutile (110) nanowires. There is a crossover in terms of energetics and bulk-like nanowires are more stable than the thin nanowires for larger radius wires after a critical diameter. These (110) rutile nanowires are all semiconductors.

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