Controlling by defects of switching of ZnO nanowire array surfaces from hydrophobic to hydrophilic

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ZnO nanowires possess structural properties, which makes them advantageous for hydrophobic applications [1]. ZnO polar and nonpolar surfaces have different wettabilities. The defects of the oxygen containing surfaces are typically responsible for interchange between hydrophilic and hydrophobic ZnO states. Understanding the atomic-level mechanisms of reversible wettability is essential for developing practical applications of ZnO wires.

We evaluated the energy reliefs of the migration of water molecules along different lateral surfaces of wires without defects and with oxygen and zinc vacancies (Fig. 1). Electric charges around atoms on the path of possible migration of water molecules were calculated using the electron density functional and pseudopotential methods from first principles using our own software code [2].

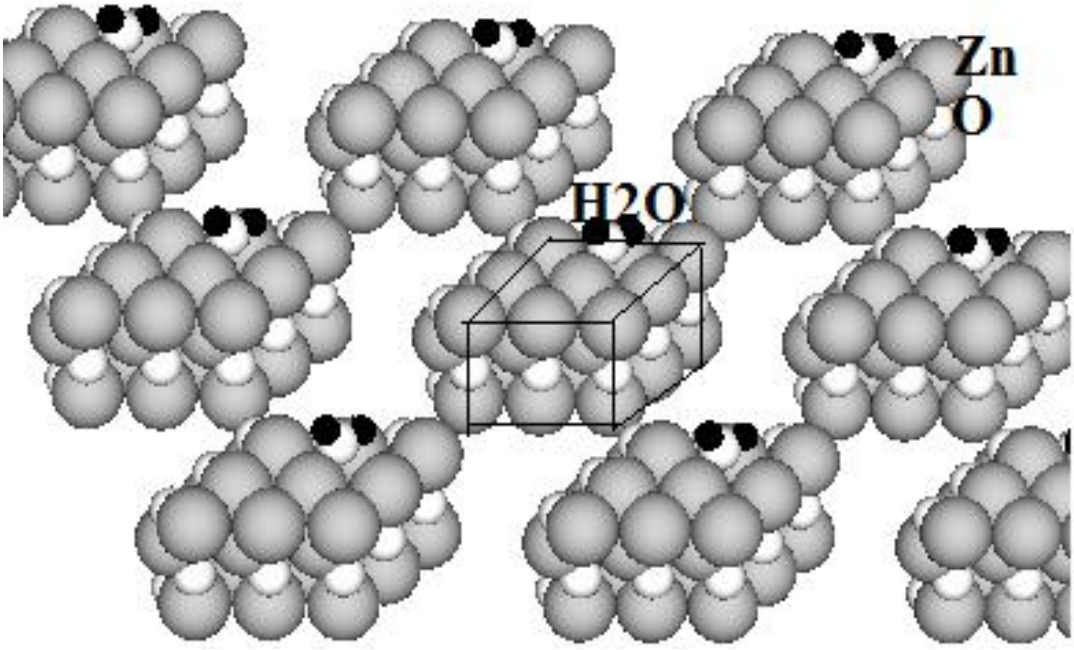

Fig. 1. Fragments of an array of ZnO wires of wurtzite crystal structure grown along the ***c***-axis: layers of Zn/O/Zn/O ions create a sequence in the [0001] direction

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