Electronic Supplementary Material (ESI) for Nanoscale Advances.

Improving Formaldehyde Sensing of ZnO Nanostructures with Surface-adsorbed oxygen

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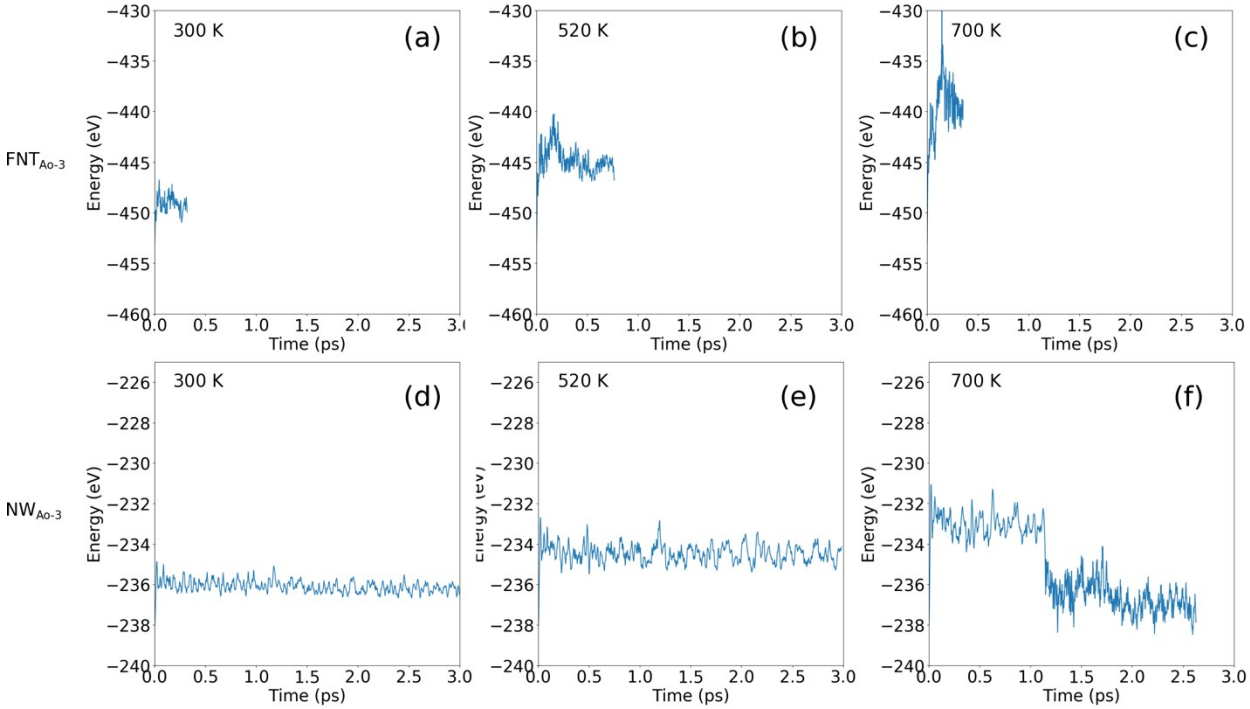

Figure S1: Evolution of the total system energy of the FNT_{Ao-3} and NW_{Ao-3} structures as function of time, by applying *ab initio* molecular dynamics, and at three temperatures: 300K, 520K and 700K. We have run the simulations in (a), (b) and (c) for shorter times because, for the case of (a), the system equilibrated to a reversible surface reaction (Equation 6), while for (b) and (c), the simulation resulted in the dissociation of the adsorbed HCO species into reaction products in their gaseous phase.