Supporting Information

Influence of the zeolite support on the catalytic properties of confined metal clusters: a periodic DFT study of O_2 dissociation on Cu_n clusters in CHA

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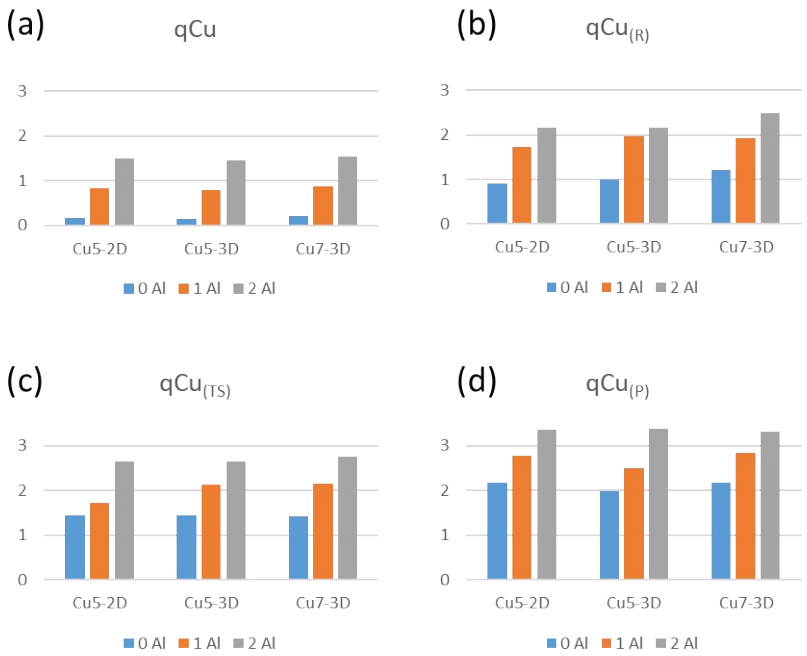

Figure S1. Total atomic charge on Cu_n clusters stabilized in CHA zeolite qCu (a) and in reactant R (b) transition state TS (c) and product P (d) structures involved in O_2 dissociation.

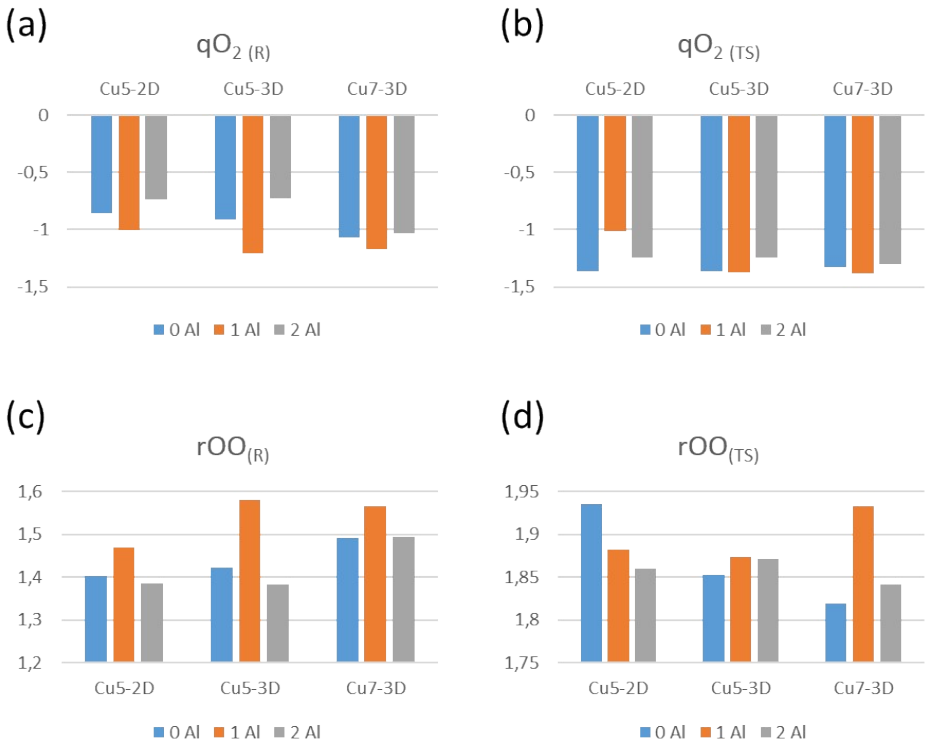

Figure S2. Total atomic charge on adsorbed O_2, qO_2, in reactant R (a) and transition state TS (b) structures, and optimized O-O distances rOO in in reactant R (c) and transition state TS (d) structures involved in O_2 dissociation.

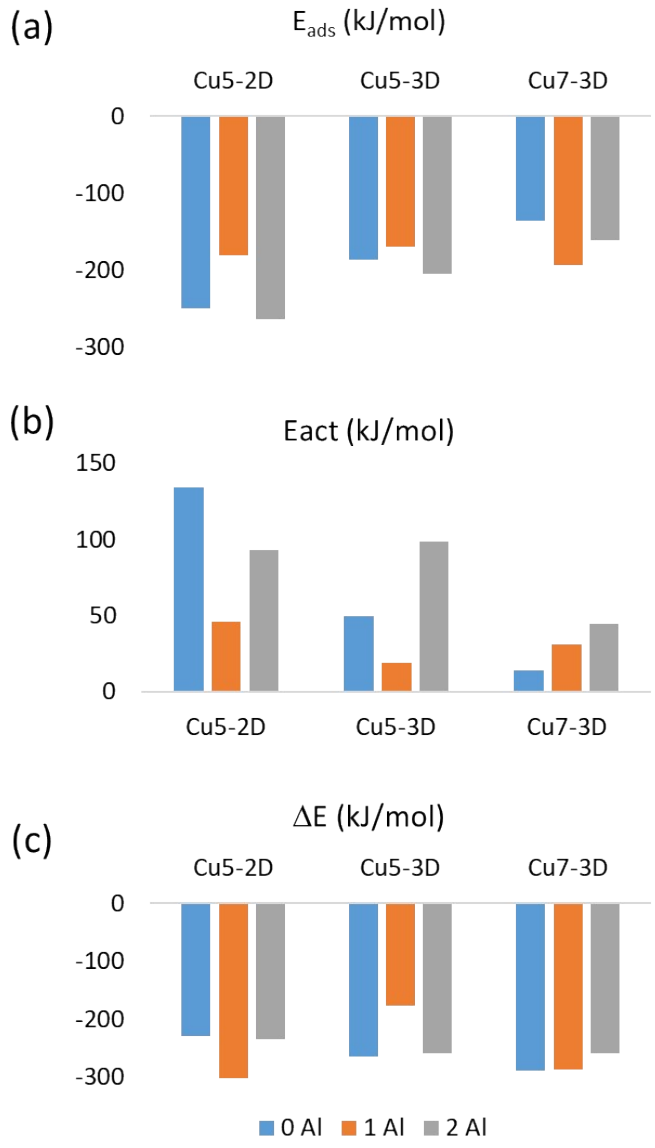

Figure S3. Calculated (a) adsorption E_{ads}, (b) activation E_{act} and (c) reaction ΔE energies (in kJ/mol) for O_2 dissociation on Cu_n clusters stabilized in CHA.

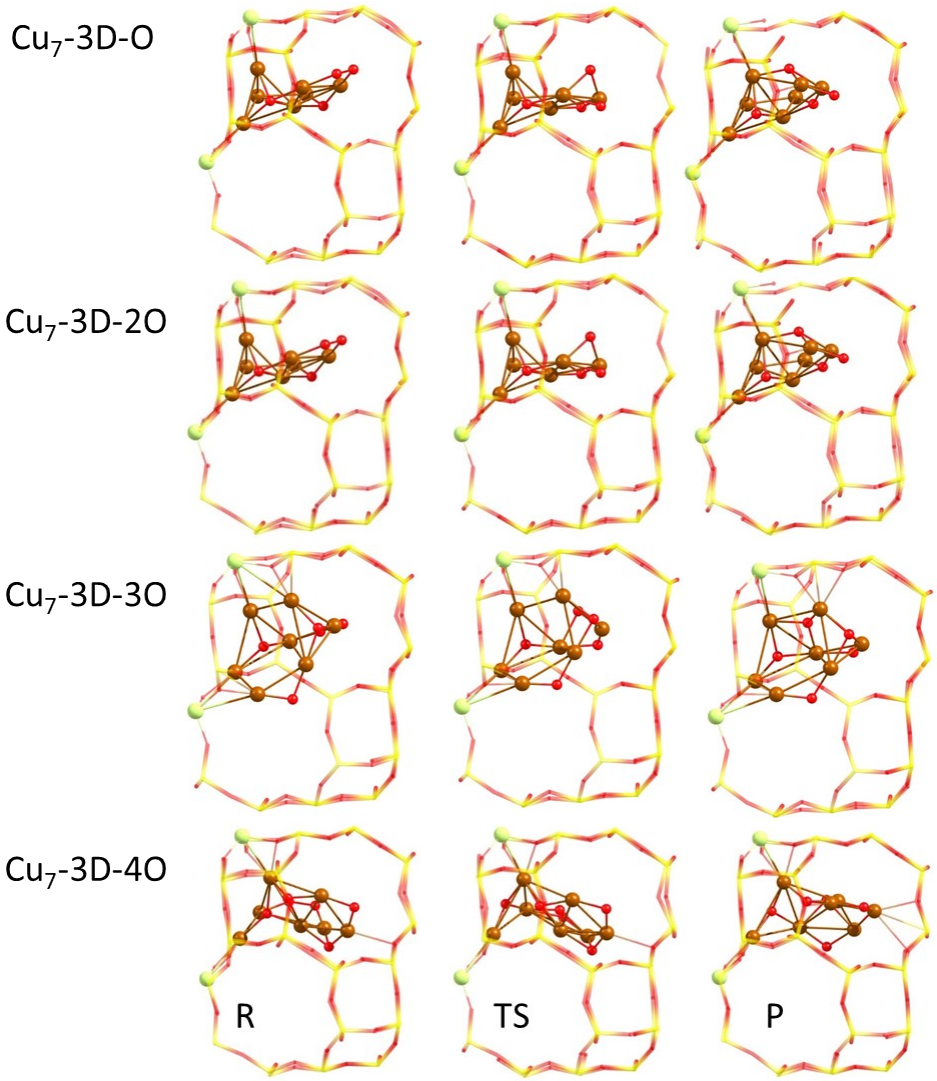

Figure S4. Optimized structures of reactant R, transition state TS and product P of O_2 dissociation reaction on Cu_7-3D-O, Cu_7-3D-2O, Cu_7-3D-3O and Cu_7-3D-4O clusters confined within CHA models with 2 framework Al atoms. Si and O are depicted as red and yellow wires, Cu and Al are depicted as brown and light green balls.