Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Unravelling the early oxidation Mechanism of zinc phosphide (Zn_3P_2) surfaces by adsorbed oxygen and water: a first-principles DFT investigation

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This supporting information contains the unrelaxed and relaxed structures of all unique terminations of the (001), (101), and (110) Zn_3P_2 surfaces. The predicted unrelaxed and relaxed surface energies are also displayed.

Figure S1: Unrelaxed and relaxed structures of the three unique terminations of Zn_3P_2 (001) surface of (Colour scheme: Zn = blue, and S = orange).

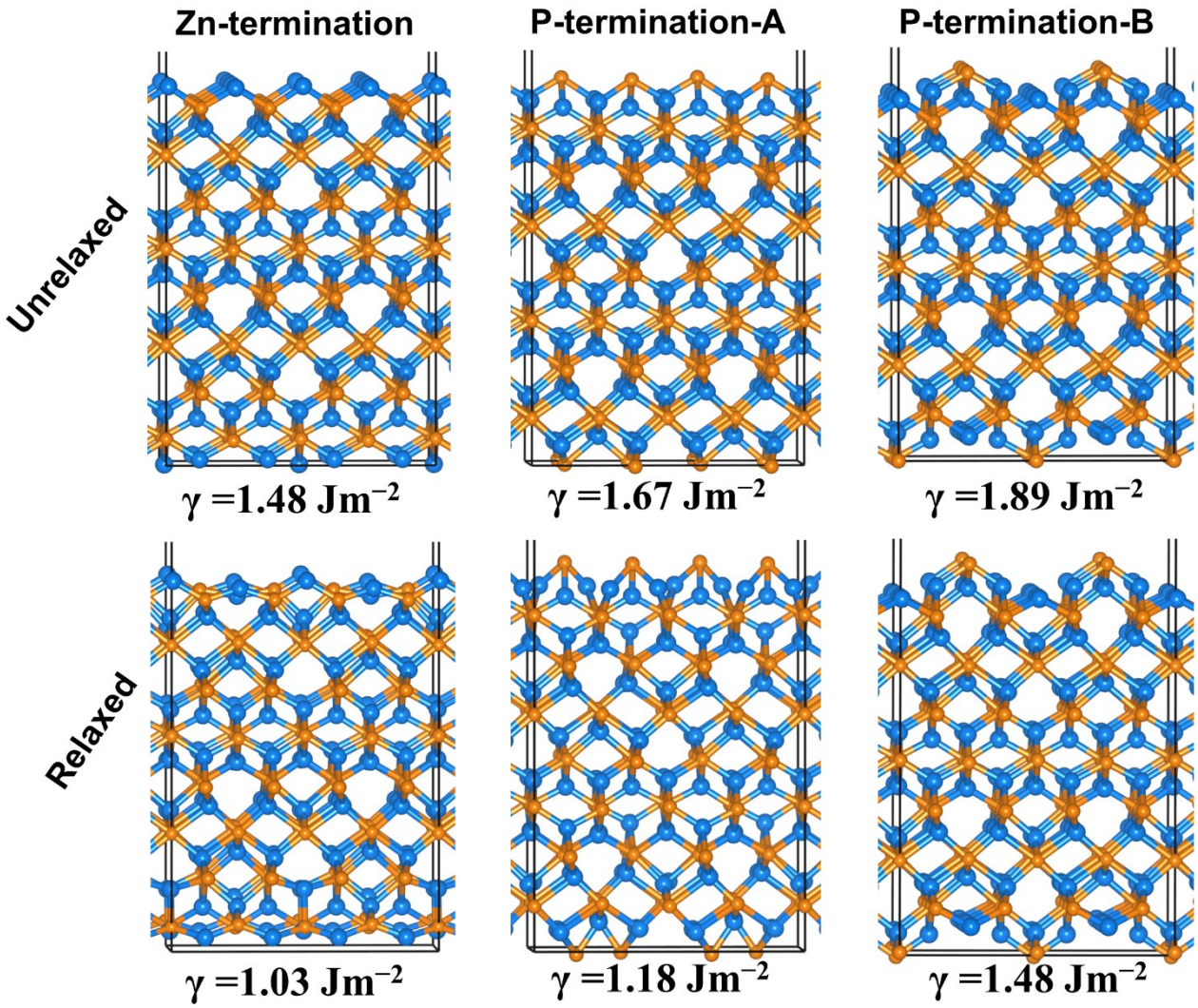

Figure S2: Unrelaxed and relaxed structures of the two unique terminations of Zn_3P_2 (101) surface of (Colour scheme: Zn = blue, and S = orange).

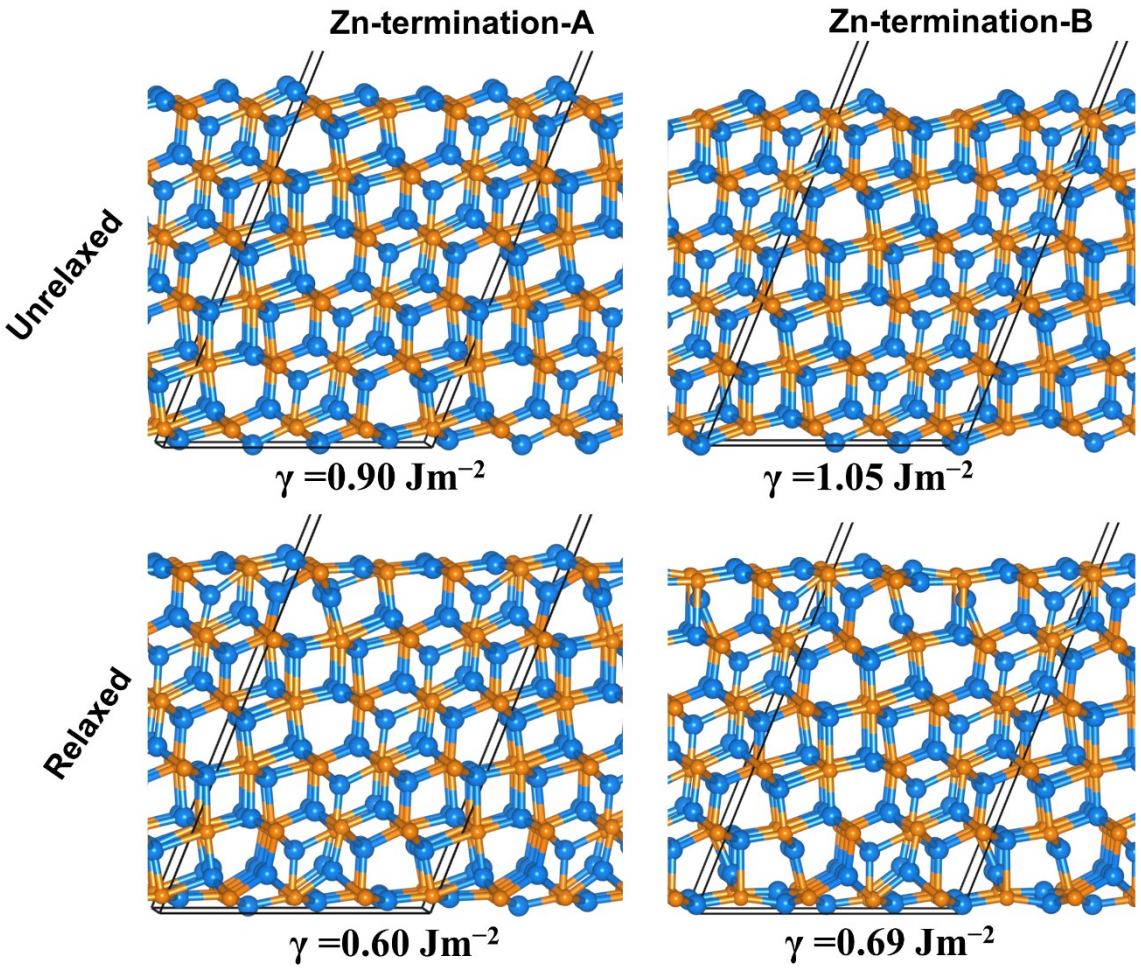

Figure S3: Unrelaxed and relaxed structures of the two unique terminations of Zn_3P_2 (110) surface of (Colour scheme: Zn = blue, and S = orange).