Supporting Information

Proposals for gas-detection improvement of FeMPc monolayer towards ethylene and formaldehyde by using bimetallic synergy

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Contents:

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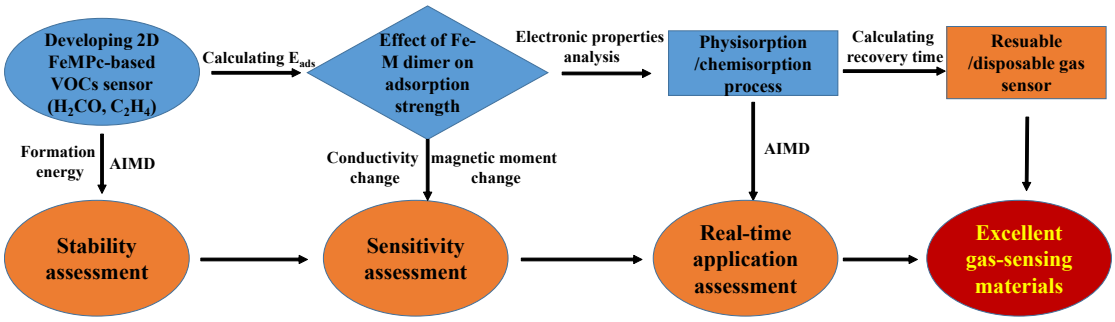
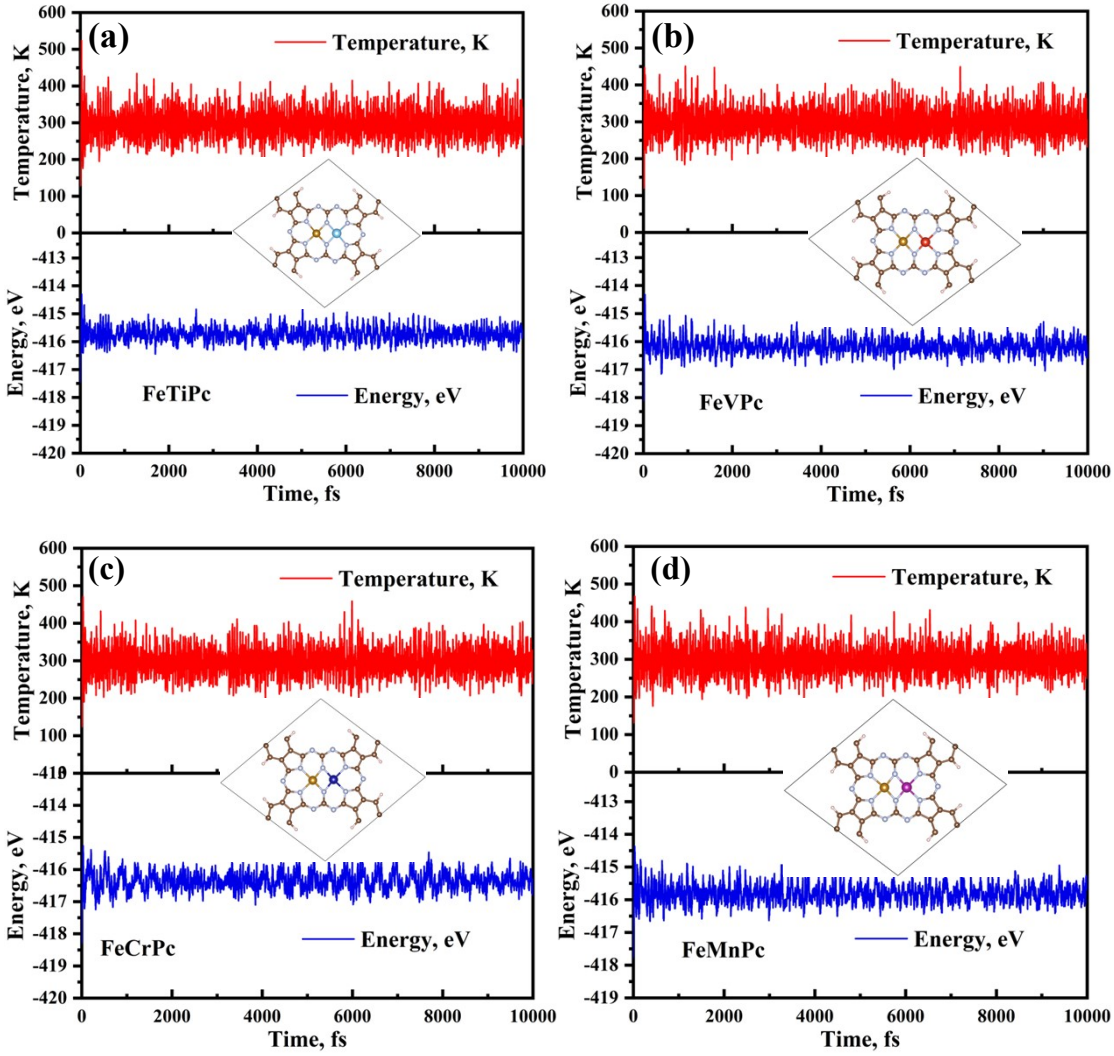


Fig. S1. Action flowchart plot of exploring 2D FeMPc (M=3d transition metal) based gas sensor for the detection of H_2CO and C_2H_4.



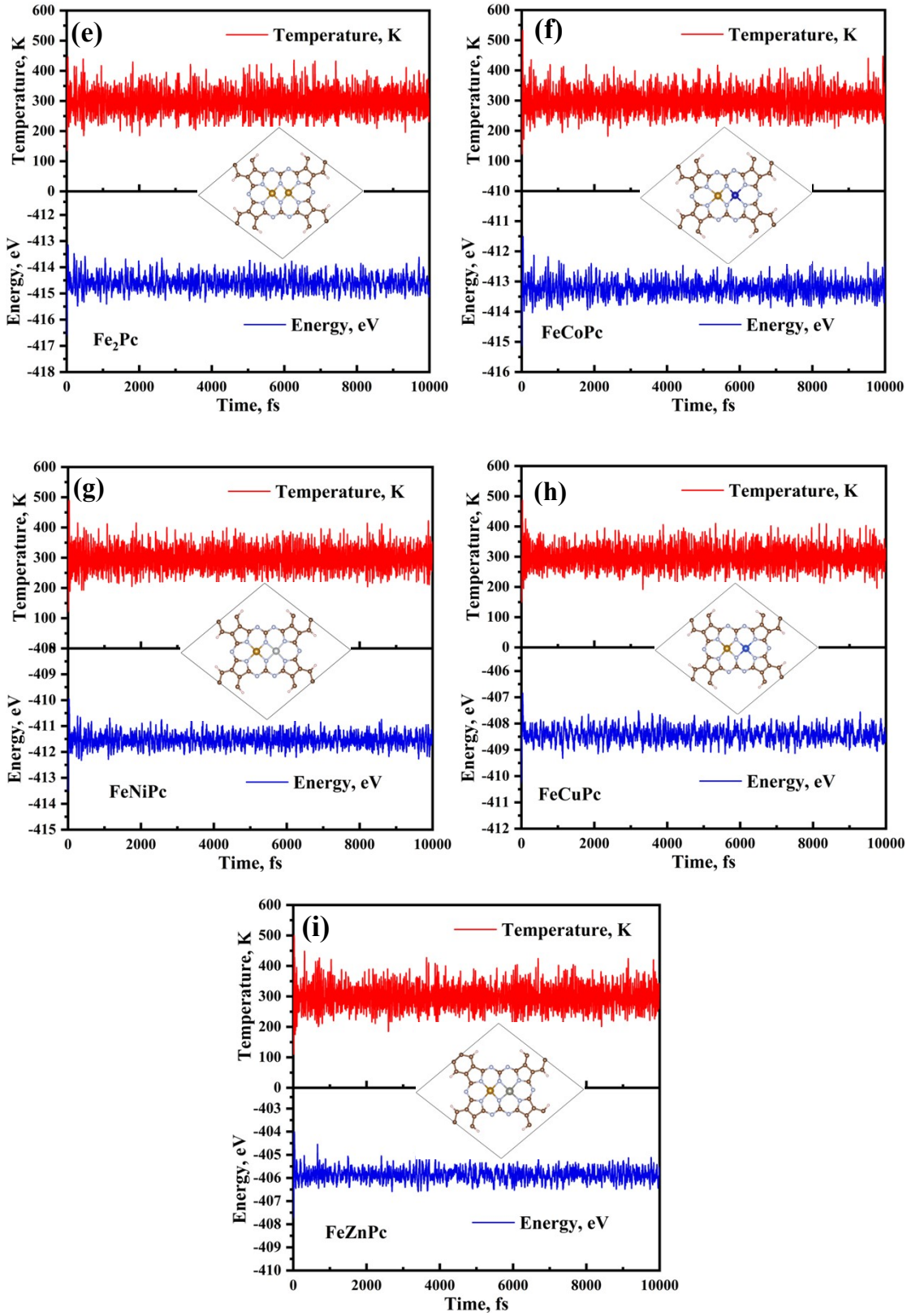


Fig. S2. Temperature and potential energy change of FeMPc monolayers in the AIMD simulations at 300 K. (a) FeTiPc, (b) FeVPc, (c) FeCrPc, (d) FeMnPc, (e) Fe2Pc, (f) FeCoPc, (g) FeNiPc, (h) FeCuPc and (i) FeZnPc.

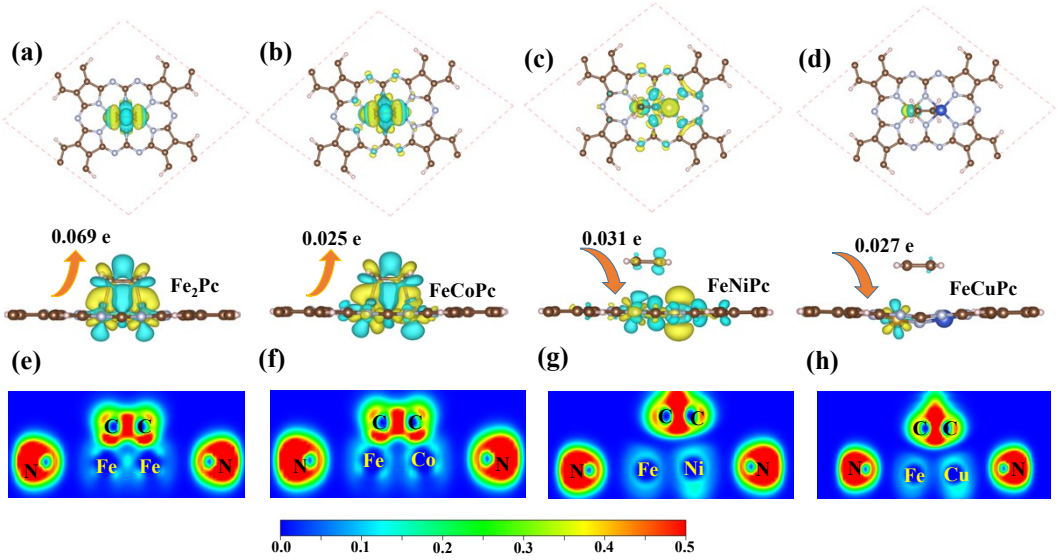


Fig. S3. cThe yellow and cyan region in CDD represent electron gain and loss, and the isosurface value is ± 0.002 e/Å^3.

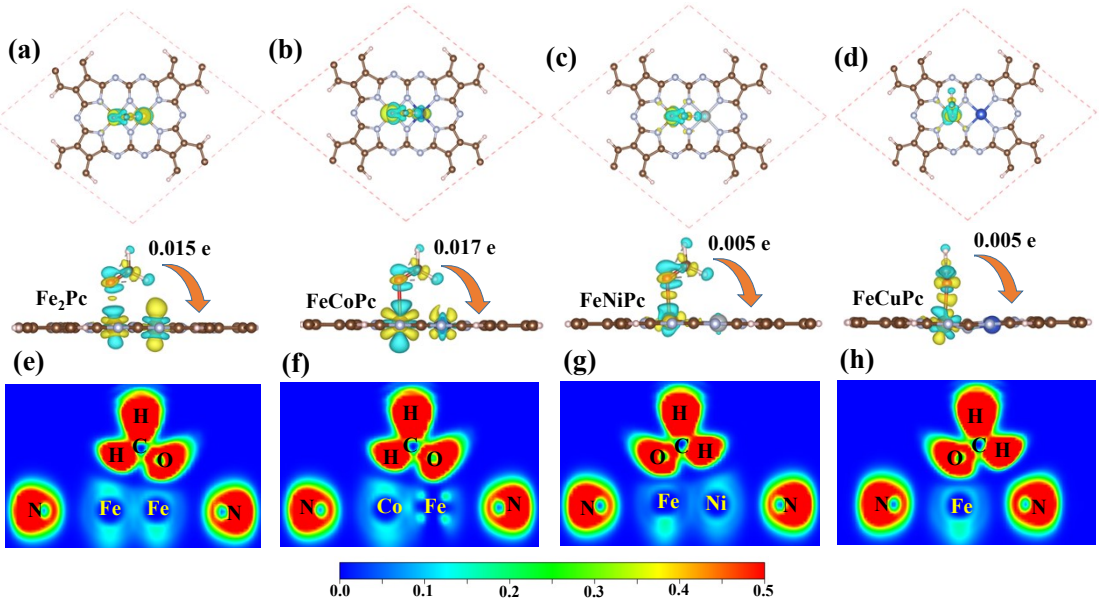


Fig. S4. (a-d) Charge density difference (CDD) and (e-h) electronic local functional (ELF) of various adsorption systems: (a) Fe_2Pc/H_2CO, (b) $FeCoPc/H_2CO$, (c) $FeNiPc/H_2CO$ and (d) $FeCuPc/H_2CO$. The yellow and cyan region in CDD represent electron gain and loss, and the isosurface value is ± 0.002 e/Å^3.

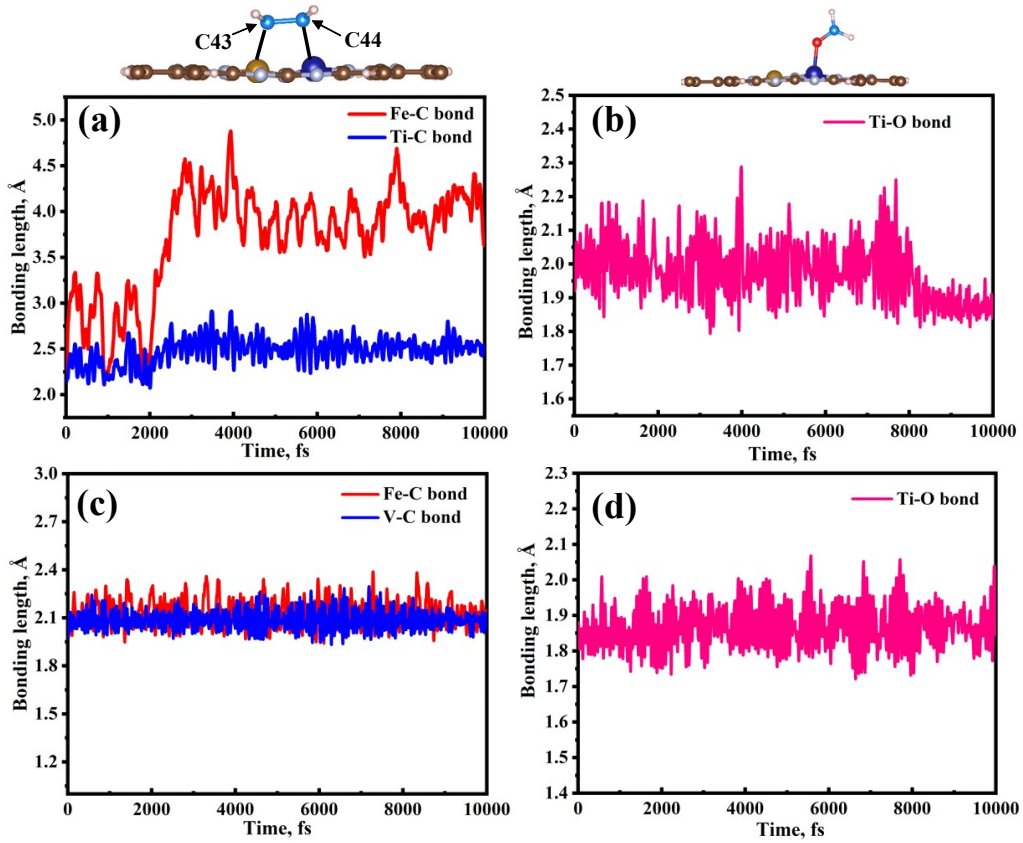


Fig. S5. Change of M-C/O bond length in different adsorption systems during the AIMD simulations at 300 K. (a) FeTiPc/C_2H_4, (b) FeTiPc/H_2CO, (c) FeVPc/C_2H_4, (d) FeVPc/H_2CO.

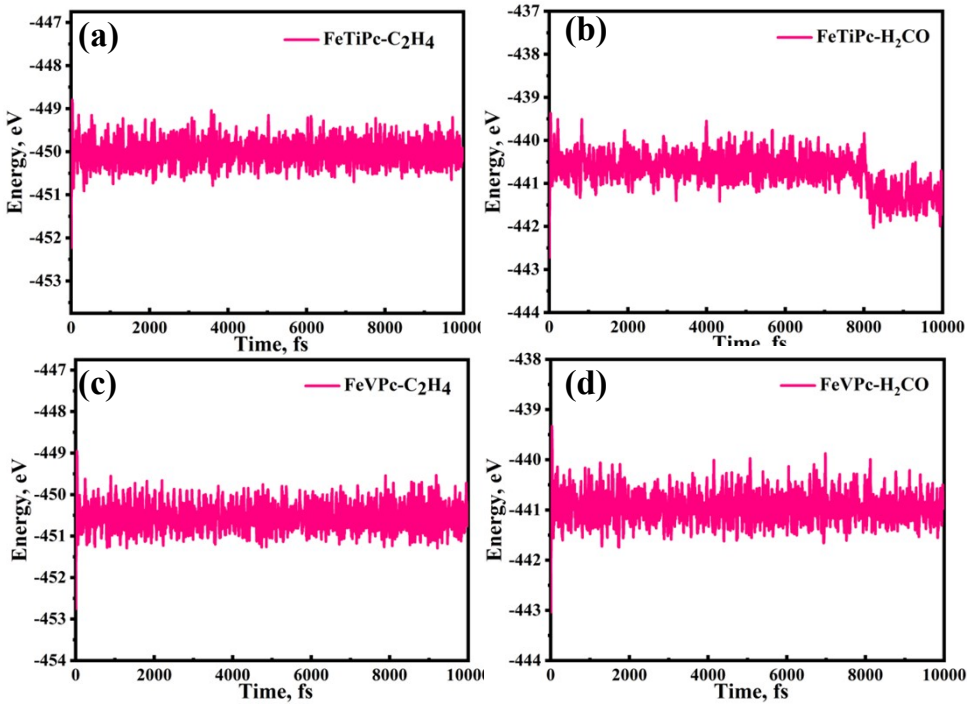


Fig. S6. Potential energy change of different adsorption systems during the AIMD simulations at 300 K. (a) FeTiPc/C_2H_4, (b) FeTiPc/H_2CO, (c) FeVPc/C_2H_4, (d) FeVPc/H_2CO.