

新型掺杂多孔芳香骨架材料的储氢性能模拟

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Simulation on the Hydrogen Storage Properties of New Doping Porous Aromatic Frameworks

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图 S1-S3 分别为 H_2 在 PAF-301、PAF- $C_4B_2H_4-Li_2-Si$ 和 PAF- $C_4B_2H_4-Li_2-Ge$ 中达到吸附平衡时的质心分布图。

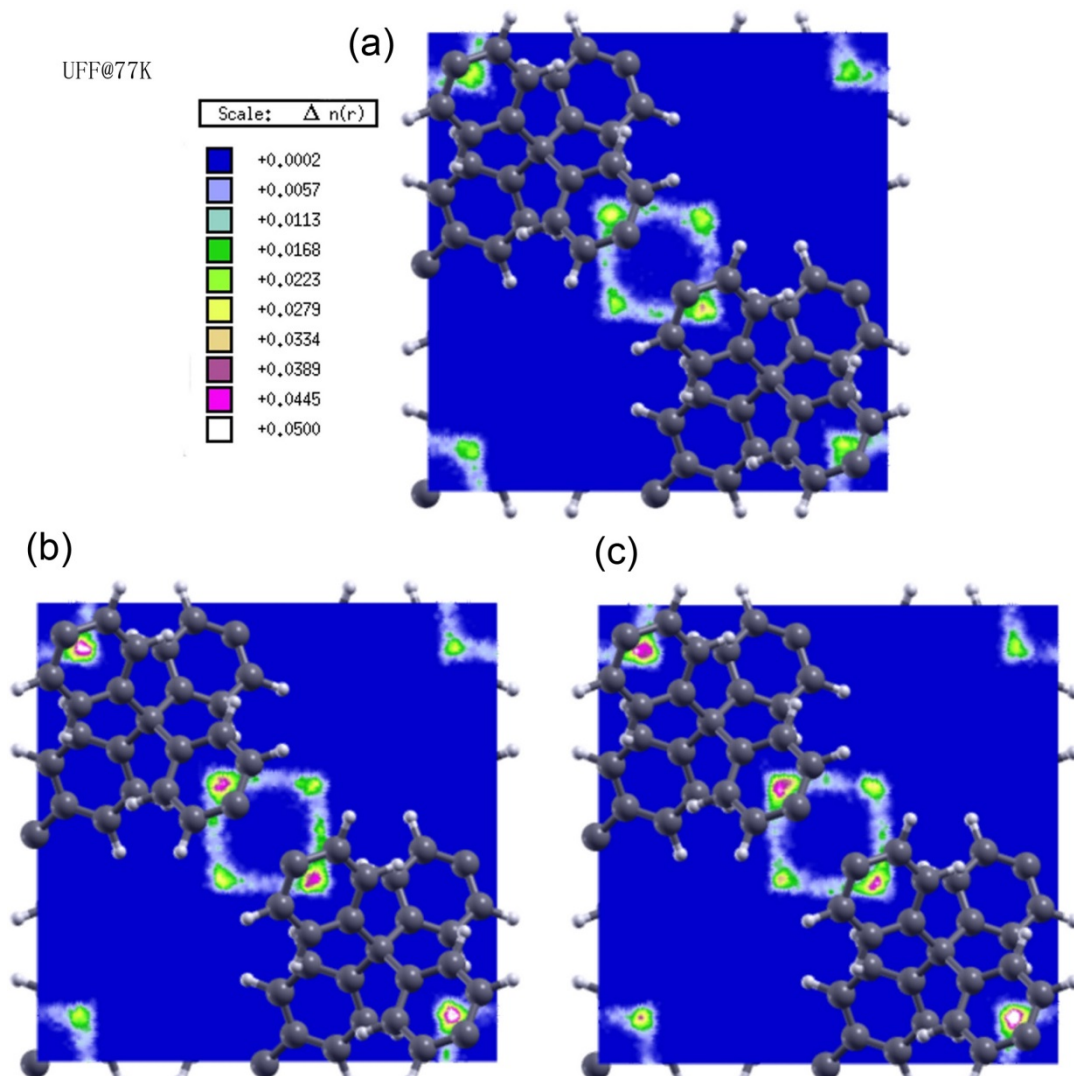


图 S1 77K 不同压力下 H_2 在 PAF-301 中吸附平衡质心密度分布
Fig.S1 Mass center density distribution (XOY) for adsorption equilibrium of H_2 on PAF-301 at various pressures and 77 K

(a) 100 kPa; (b) 3.5 MPa; (c) 7.0MPa. $\Delta n(r)$ in the thermometer is dimensionless.

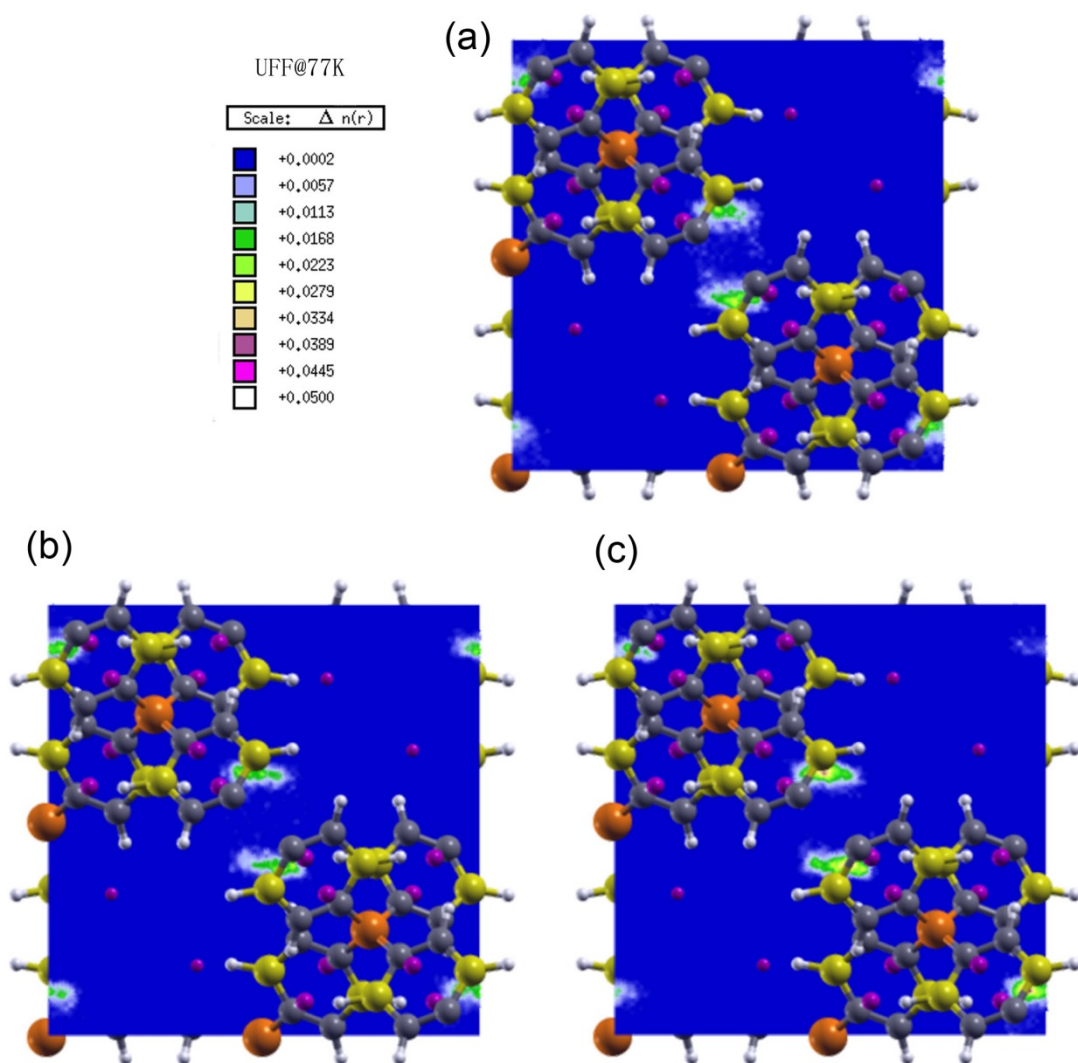


图 S2 77K 不同压力下 H_2 在 PAF-C4B2H4-Li₂_Si 中吸附平衡质心密度分布
 Fig.S2 Mass center density distribution (XOY) for adsorption equilibrium of H_2 on
 PAF-C4B2H4-Li₂_Si at various pressures and 77 K

(a) 100 kPa; (b) 3.5 MPa; (c) 7.0 MPa. $\Delta n(r)$ in the thermometer is dimensionless.

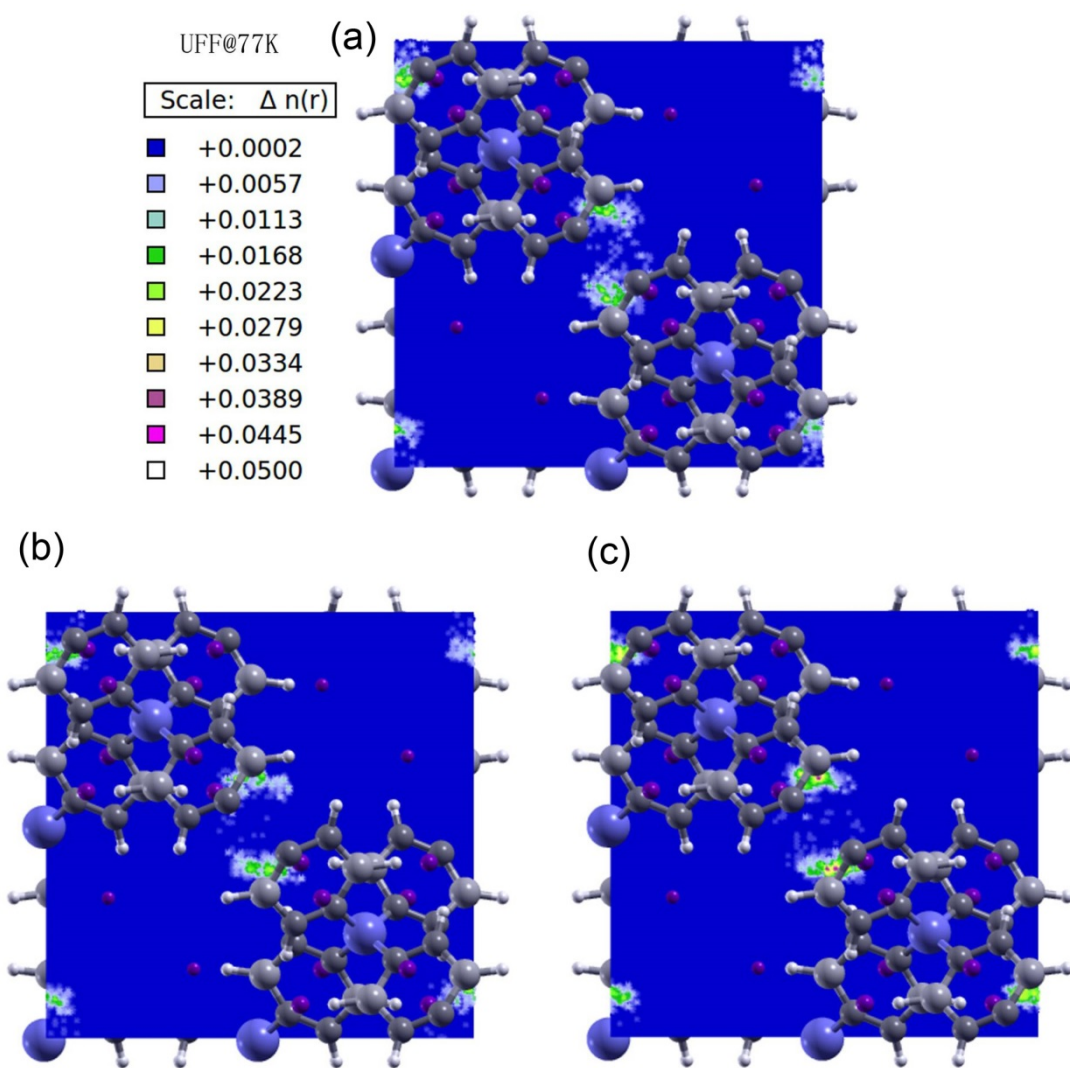


图 S3 77K 不同压力下 H_2 在 PAF-C4B2H4-Li₂_Ge 中吸附平衡质心密度分布
 Fig.S3 Mass center density distribution (XOY) for adsorption equilibrium of H_2 on
 PAF-C4B2H4-Li₂_Ge at various pressures and 77 K

(a) 100 kPa; (b) 3.5 MPa; (c) 7.0 MPa. $\Delta n(r)$ in the thermometer is dimensionless.