

## Supplementary Data

### DFT Study of Pd-doped $\text{ZrCl}_2$ : A Promising Solution for Dissolved Gas Molecules Analysis in Transformer Oil

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- Study into the adsorption properties of targeted gases on Vacant  $\text{ZrCl}_2$  ML:

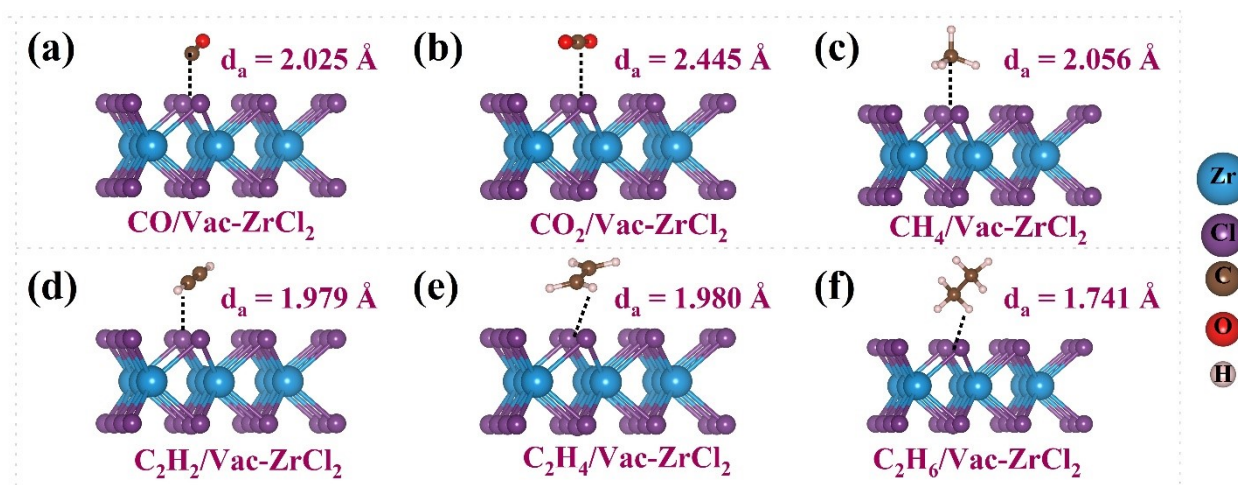


Figure S1: Stable structure of all gas molecules on Vacant  $\text{ZrCl}_2$  ML

**Table-S1:** Adsorption energies  $E_{\text{ads}}$  (eV), Adsorption distance  $d$  (Å), of gas molecules adsorbed on the Vacant  $\text{ZrCl}_2$  ML

System	CO	CO <sub>2</sub>	CH <sub>4</sub>	C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>
Vacancy on $\text{ZrCl}_2$ ML						
$d_a$ (Å)	2.025	2.445	2.056	1.979	1.980	1.741
$E_{\text{ads}}$ (eV)	-0.174	-0.197	-0.173	-0.195	-0.235	-0.234

- **Spin-polarized Density of States:**

The spin-polarized density of states (DOS) for the pristine  $\text{ZrCl}_2$  and Pd- $\text{ZrCl}_2$  MLs reveal no noticeable spin-splitting between the up-spin and down-spin channels. This indicates that

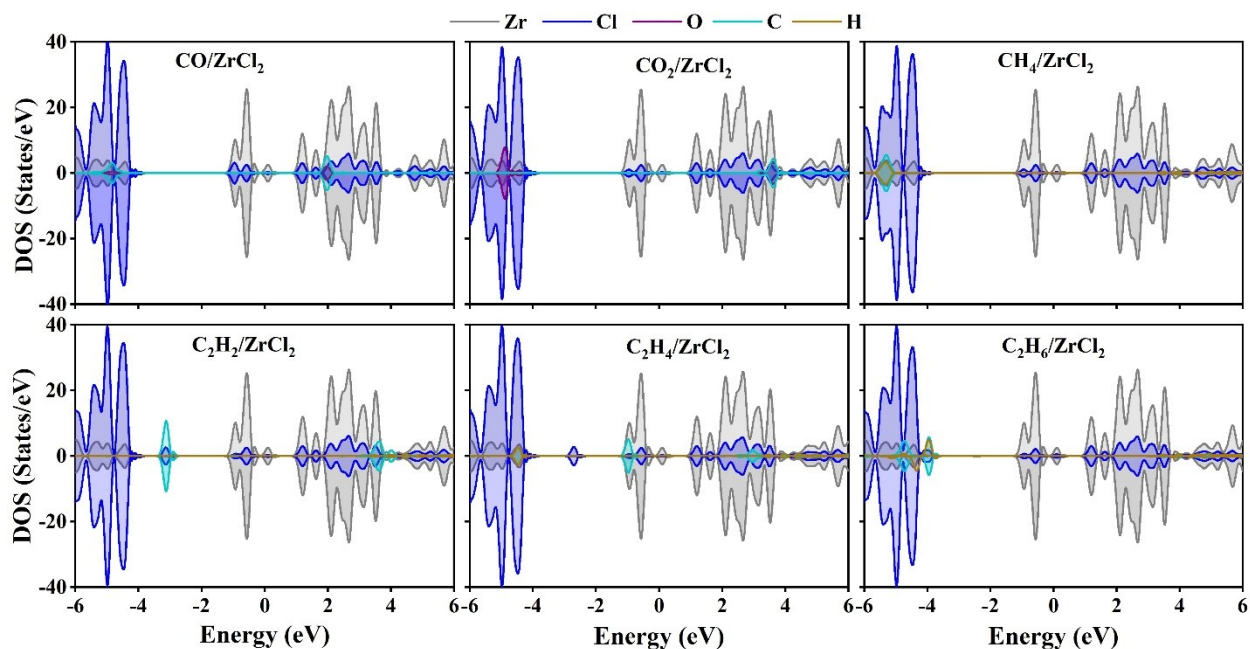


Figure S2(a): Spin-polarized DOS of all gases on  $\text{ZrCl}_2$  ML

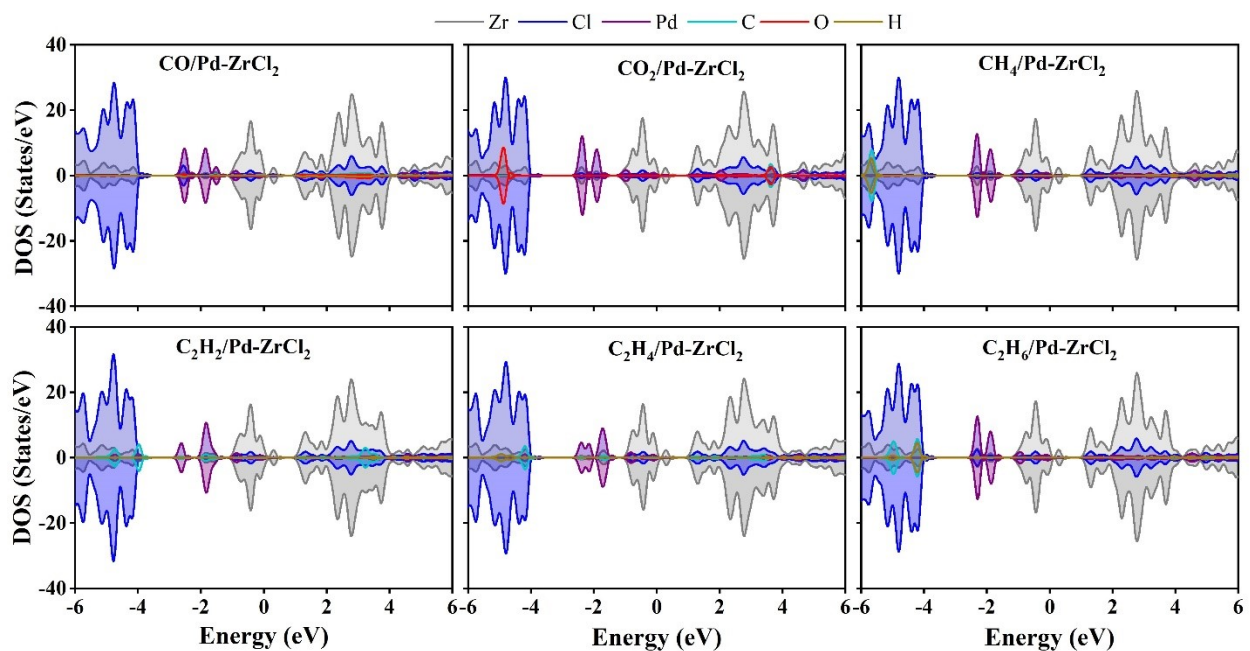


Figure S2(b): Spin-polarized DOS of all gases on Pd- $\text{ZrCl}_2$  ML

the material is non-magnetic, justifying the exclusion of spin effects in adsorption energy calculations.