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Supplementary Information

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Figure S1. Possible adsorption sites of gas molecules on the central Mn atom of MnPc molecule.

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	1	2	3	4	5	6
СО	-8675.106	-8673.597	-8674.266	-8674.262	-8674.265	
NO	-8788.386	-8786.789	-8788.158	-8786.257	-8788.157	
O ₂	-8949.474	-8949.476	-8949.877			
CO ₂	-9110.242	-9110.248	-9110.308	-9110.321		
NO ₂	-9221.891	-9221.359	-9221.893	-9221.435	-9221.895	-9221.434
NH3	-8403.451	-8403.044				

Table S1. Total energy of the corresponding adsorption structures as shown in Figure S1. The unit is eV.

The red denotes the minimum energy.