

The Structural and Surface Modification of Zeolitic Imidazolate Framework Towards Reduction of Encapsulated CO₂

Soumitra Payra¹, Swapna Challagulla¹, Ramesh Reddy Indukuru²,
Chanchal Chakraborty¹, Kartick Tarafder², Balaram Ghosh³, Sounak Roy^{1*}

¹Department of Chemistry, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus,
Jawahar Nagar, Shameerpet Mandal, Hyderabad-500078, India

²Department of Physics, National Institute of Technology Karnataka, Surathkal, Mangalore, 575 025,
Karnataka, India.

³ Department of Pharmacy, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus,
Jawahar Nagar, Shameerpet Mandal, Hyderabad-500078, India

Fig. S1. XRD patterns of ZIF-8 (CH, NH₃-25, 100, 200).

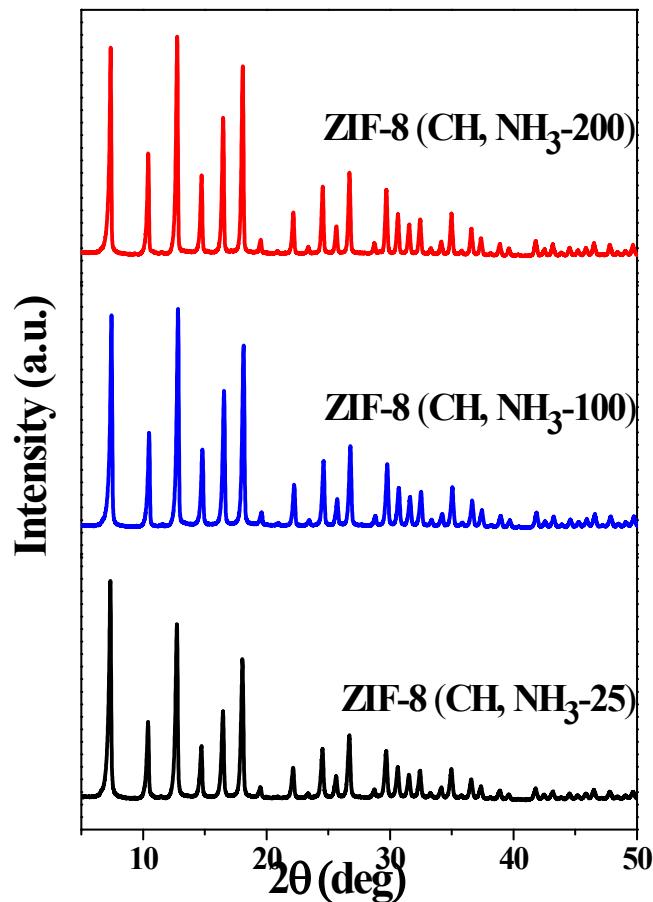


Fig. S2. *In situ* temperature XRD patterns of (a) ZIF-8 (MH), and (b) ZIF-8 (CH, NH₃-200) (# indicates (100) (002) (101) (102) planes of ZnO).

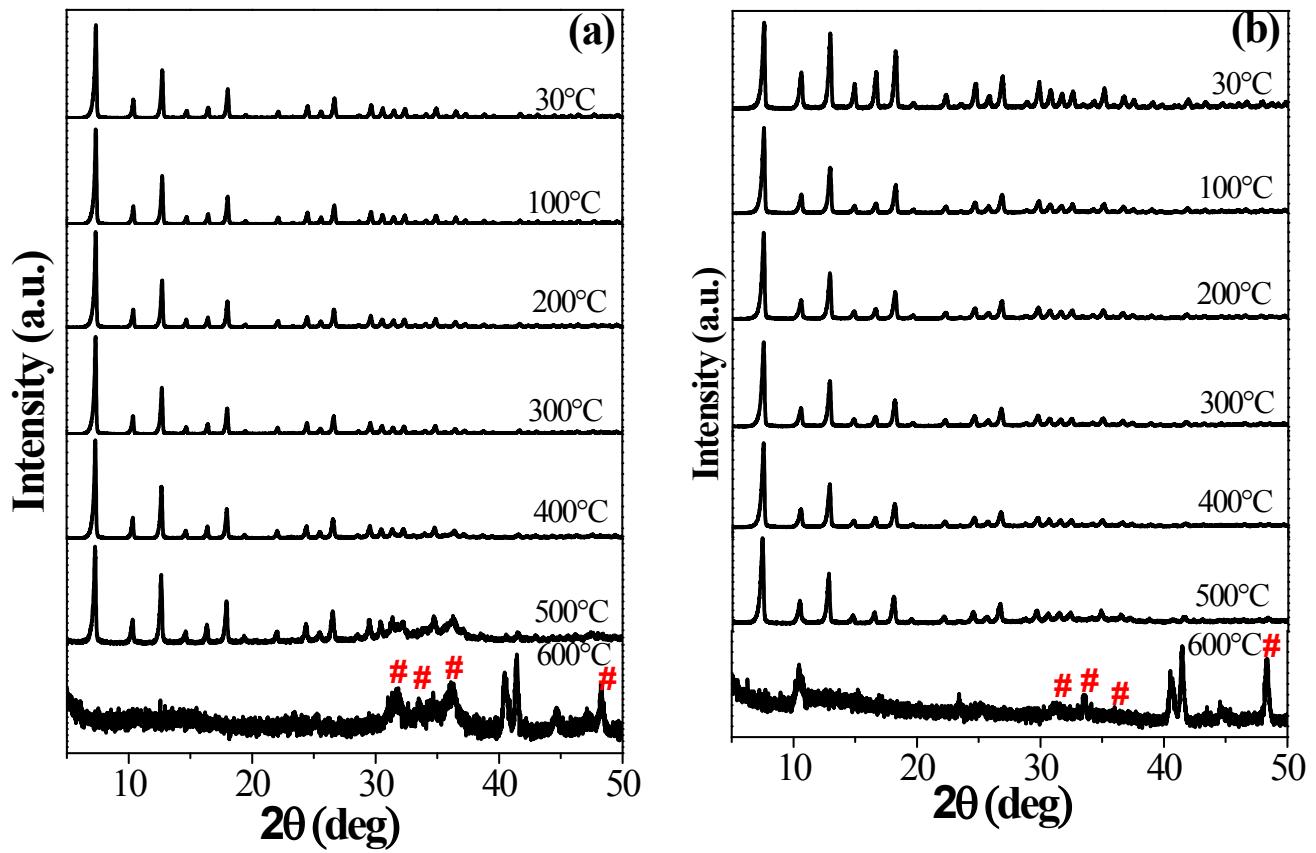


Fig. S3. (a) The LCMS data showing presence of NH₄OH in water after TGA of ZIF-8 (CH, NH₃-200), (b) FTIR of ZIF-8 (MH), calcined and as-prepared ZIF-8 (CH, NH₃-200).

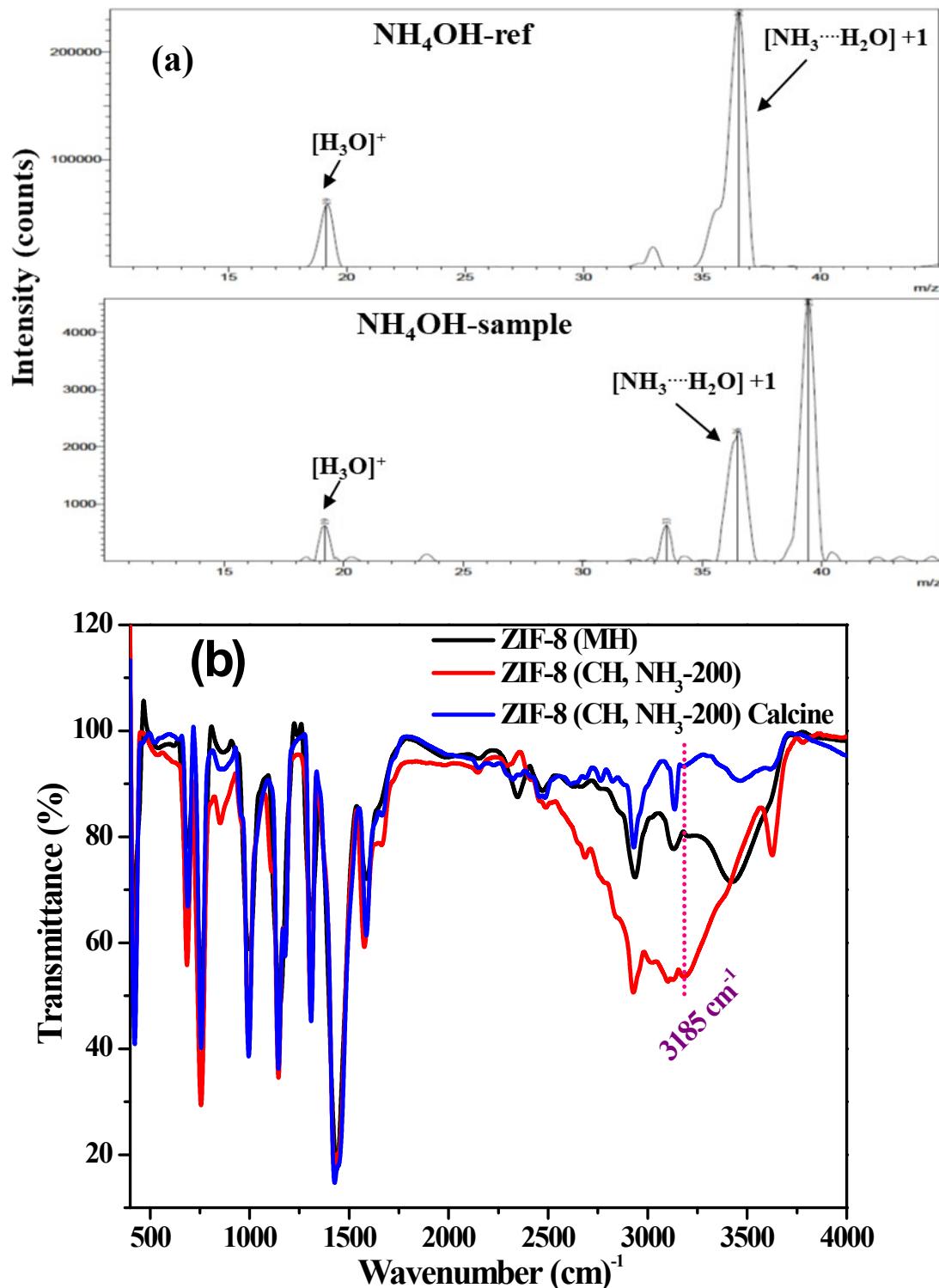


Fig. S4. The particle size distribution of (a) ZIF-8 (MH) and (b) ZIF-8 (CH, NH₃-200), and FE-SEM images of (c,d,e) ZIF-8 (CH, NH₃-25), and (f,g,h) ZIF-8 (CH, NH₃-100).

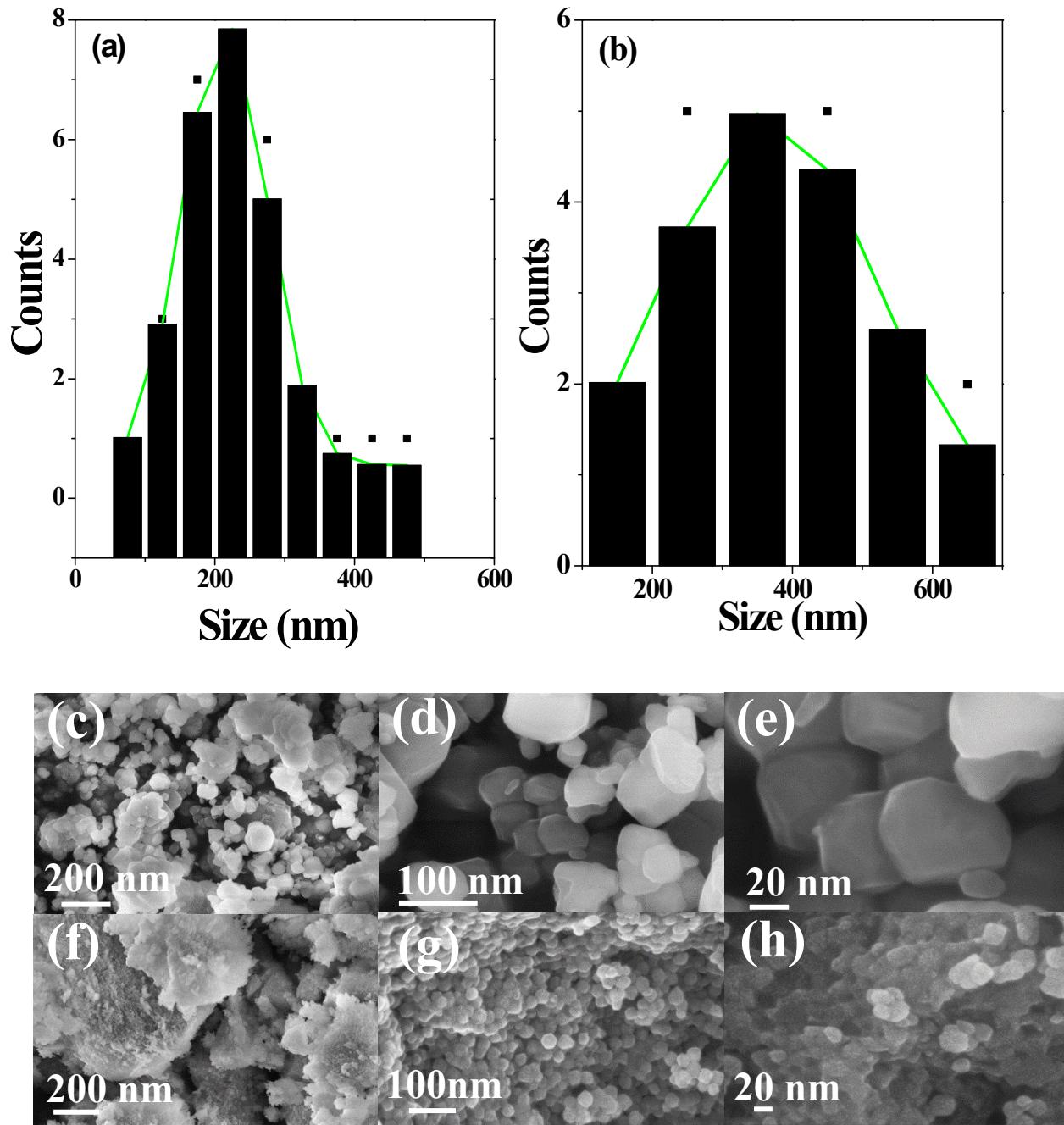


Fig. S5. N₂ adsorption-desorption of (a) ZIF-8 (CH, NH₃-25), and (b) ZIF-8 (CH, NH₃-100), (c) BET fitting, (d) Langmuir fitting, (e) adsorption – desorption profile in log scale, and (f) pore size distribution of the synthesized catalysts.

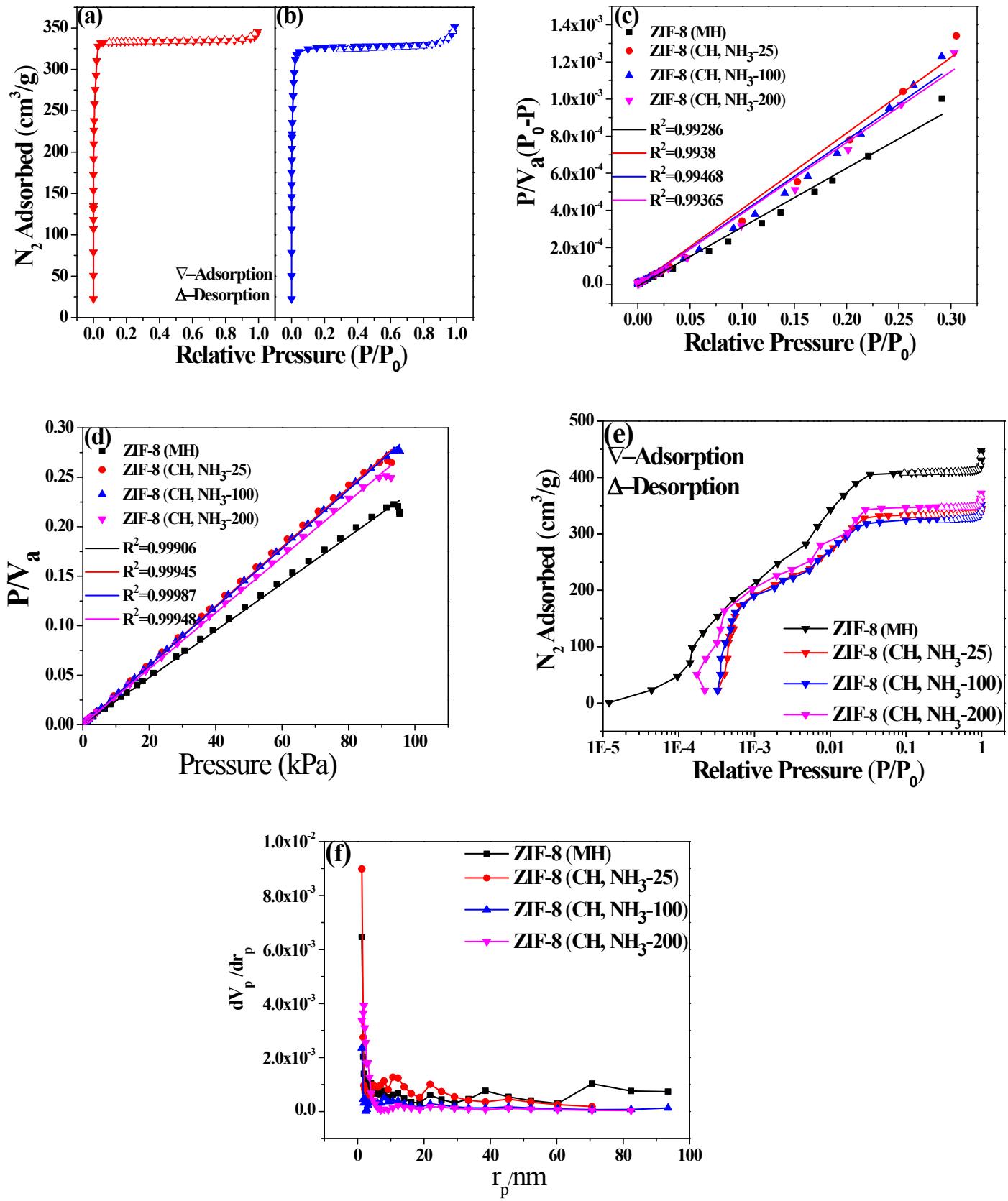


Fig. S6. Langmuir fitting of experimentally observed CO₂ adsorption-desorption profile of (a) ZIF-8 (MH) and (b) ZIF-8 (CH, NH₃-200).

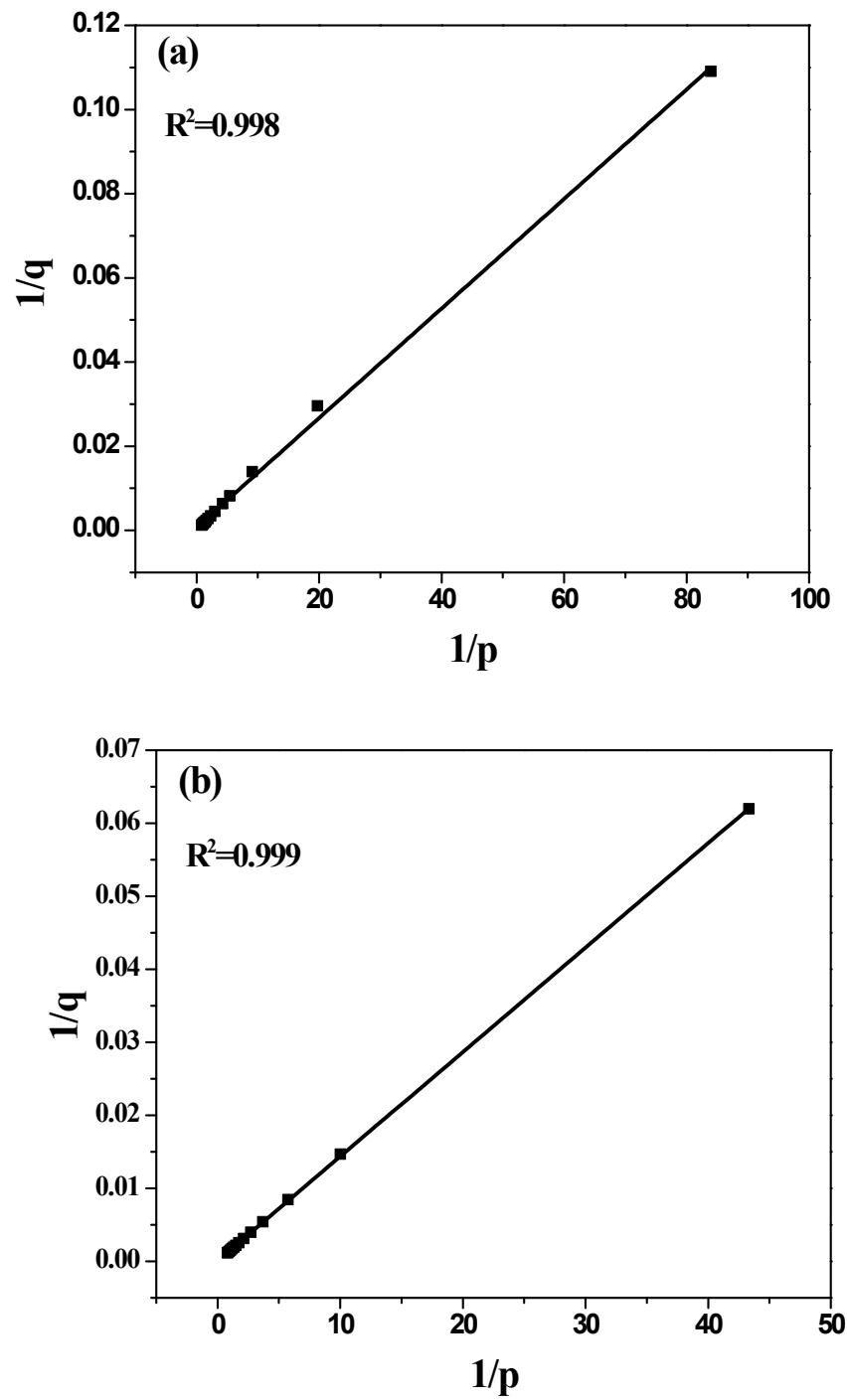


Fig. S7. Variation scan rate study of (a,b) ZIF-8 (MH), (c,d) ZIF-8 (CH, NH₃-200).

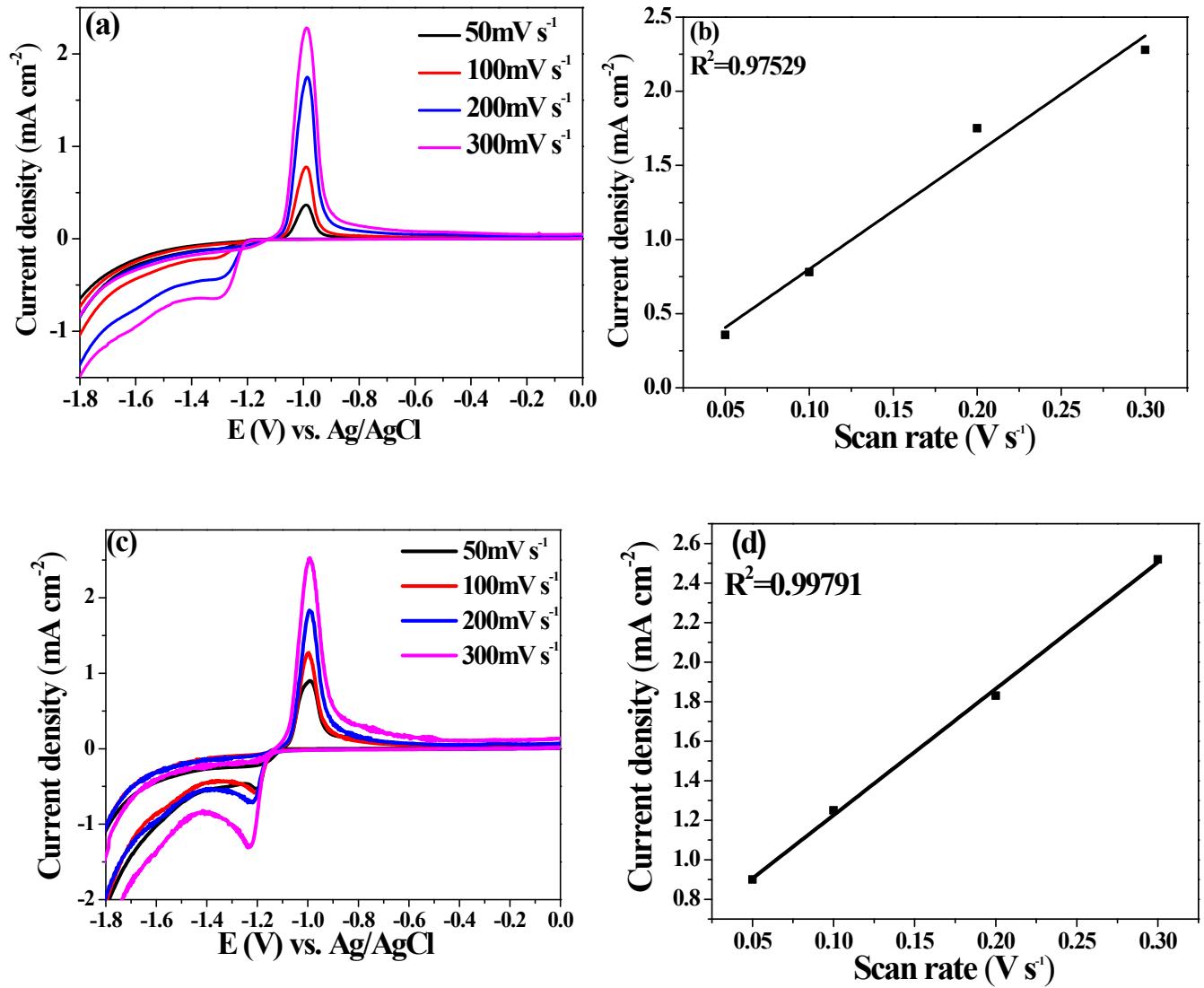


Table. S1.

Material	BET surface area (m ² g ⁻¹)	Langmuir surface area (m ² g ⁻¹)	Total pore volume(cm ³ g ⁻¹)	Mean pore size(Å)
ZIF-8 (CH, NH ₃ -25)	1287.5	1448.3	0.543	16.87
ZIF-8 (CH, NH ₃ -100)	1288.7	1458	0.530	16.40