



A Bifunctionalised Pb-Based MOF for Iodine Capture and Dyes Removal

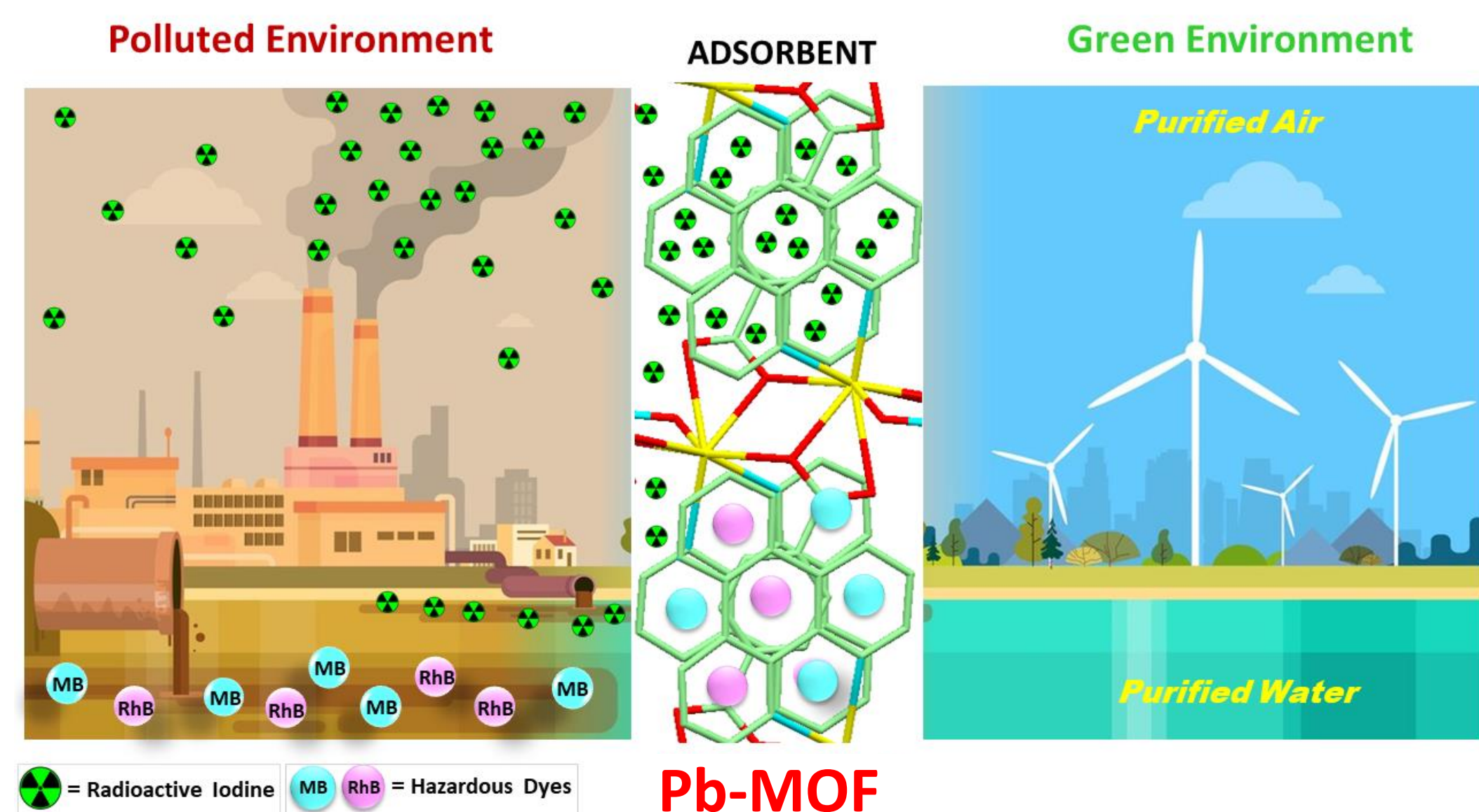
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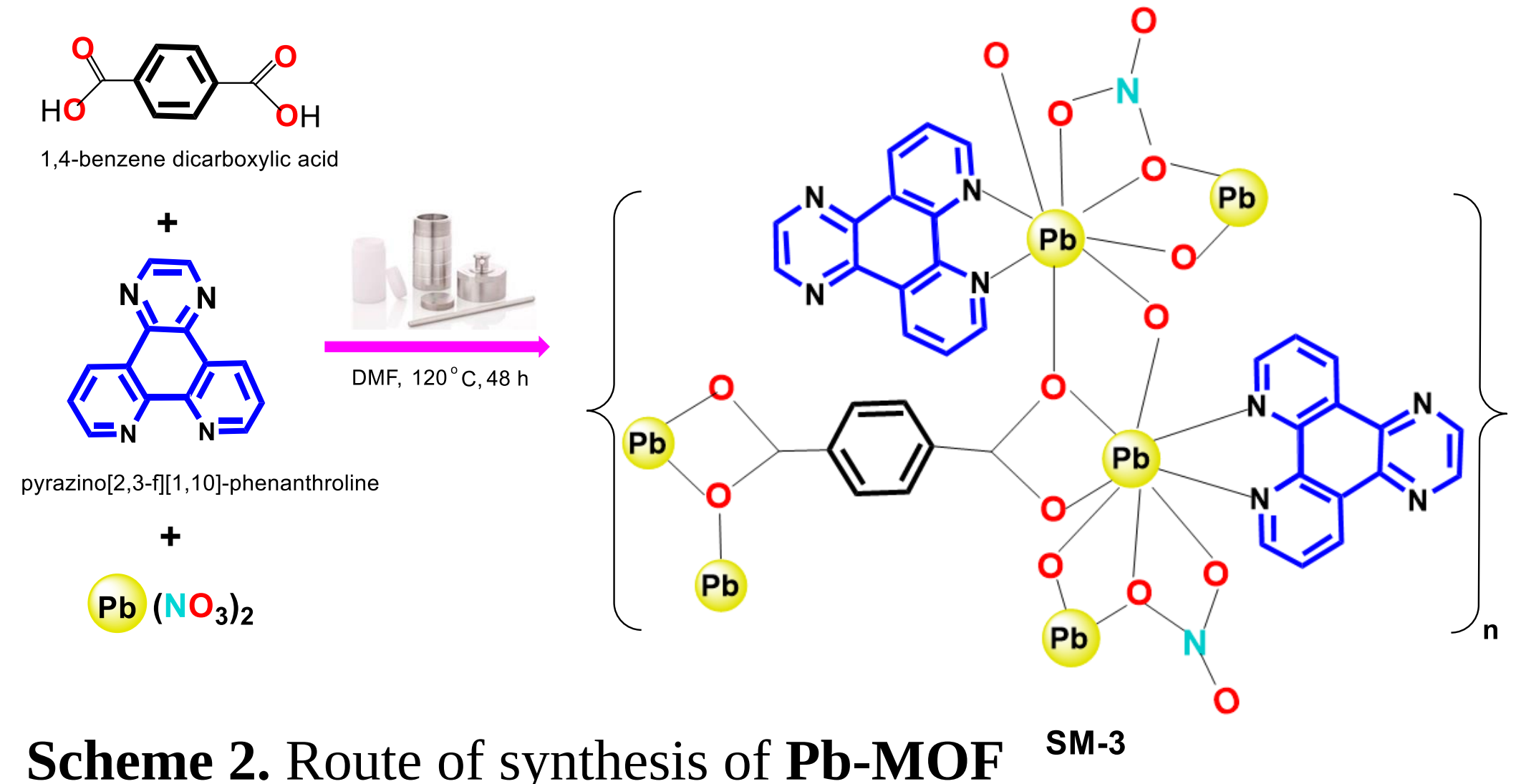
1 INTRODUCTION

- Research on clean, safe energy sources has been flourishing rapidly to meet the increasing energy demands globally and promptly reduce greenhouse emissions.
- Radioactive iodine must be adsorbed immediately after release to prevent environmental pollution due to its high volatility and easy diffusion.
- On the other hand, water pollution due to harmful chemicals, mainly organic dyes, causes serious problems for flora and fauna.
- Recently, metal-organic frameworks (MOFs) have emerged as potential candidates to adsorb radioactive iodine and dyes.



Scheme 1. Designed Pb-MOF act as an adsorbent for Iodine and Dyes.

2 Synthetic Scheme



Scheme 2. Route of synthesis of Pb-MOF

3 Characterization

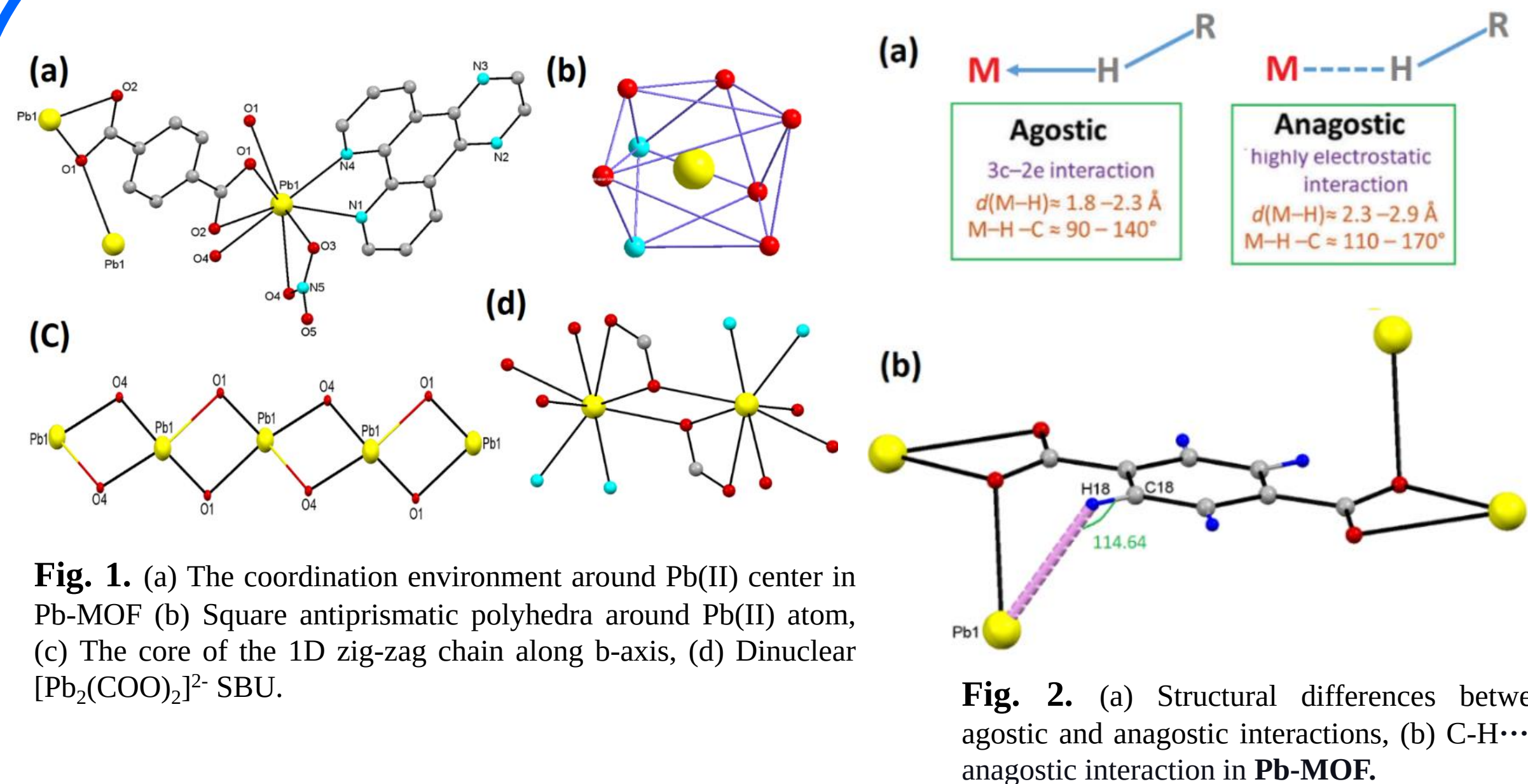


Fig. 1. (a) The coordination environment around Pb(II) center in Pb-MOF (b) Square antiprismatic polyhedra around Pb(II) atom, (c) The core of the 1D zig-zag chain along b-axis, (d) Dinuclear [Pb₂(COO)₂]²⁻ SBU.

Fig. 2. (a) Structural differences between agostic and anagostic interactions, (b) C-H...Pb anagostic interaction in Pb-MOF.

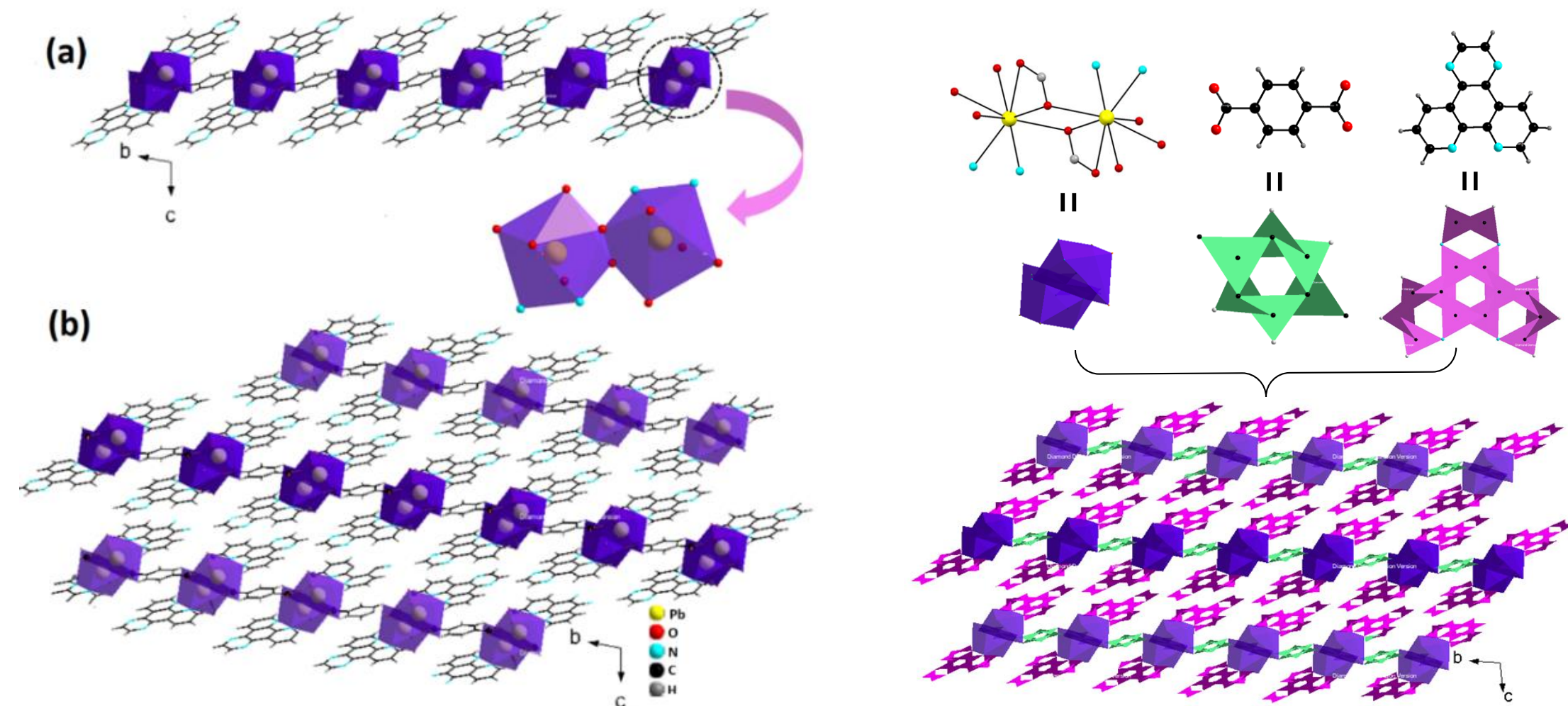


Fig. 3. Combination of dinuclear SBUs, bdc²⁻ and ph-Phen ligands results in the formation of 2D framework of Pb-MOF.

4 Iodine Capture in Vapor

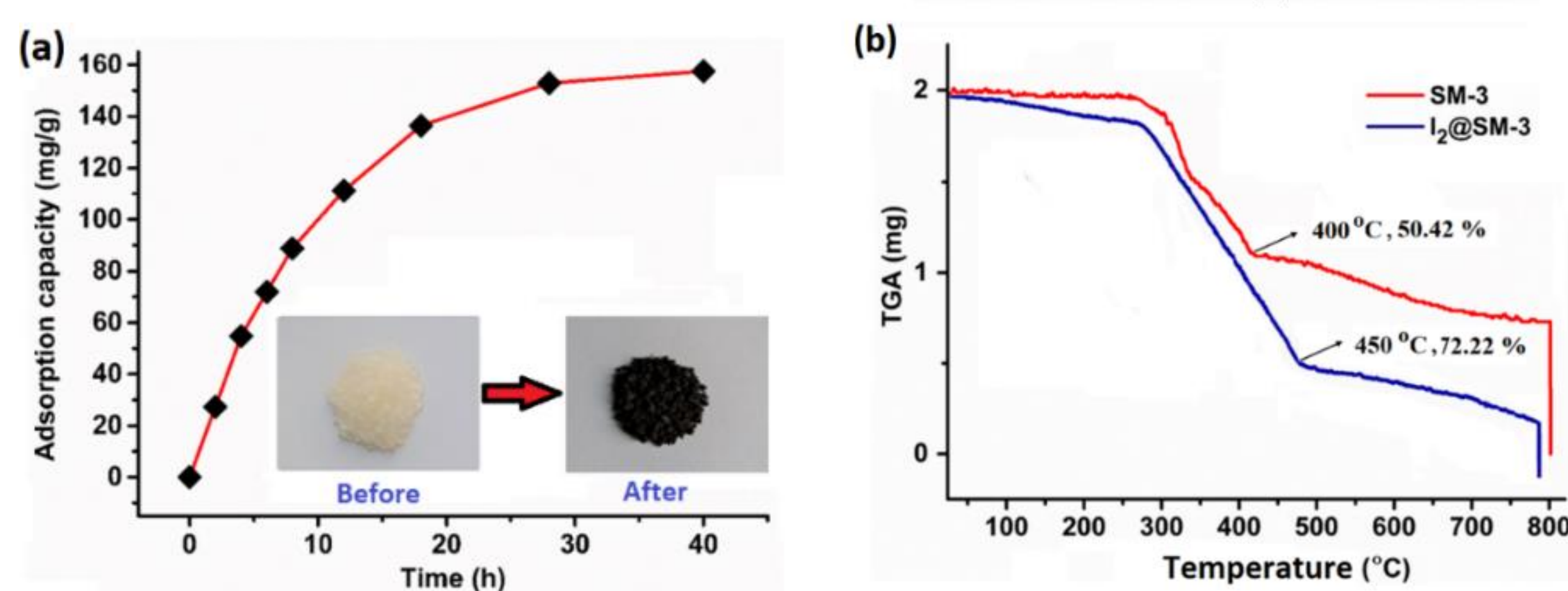


Fig. 4. (a) Change in the adsorbed amount of I₂ by Pb-MOF relative to time (inset: photographs of SM-3 crystals before and after I₂ adsorption). (b) TGA curves of Pb-MOF and I₂@Pb-MOF before and after iodine adsorption, respectively.

5 Iodine Capture in Solution

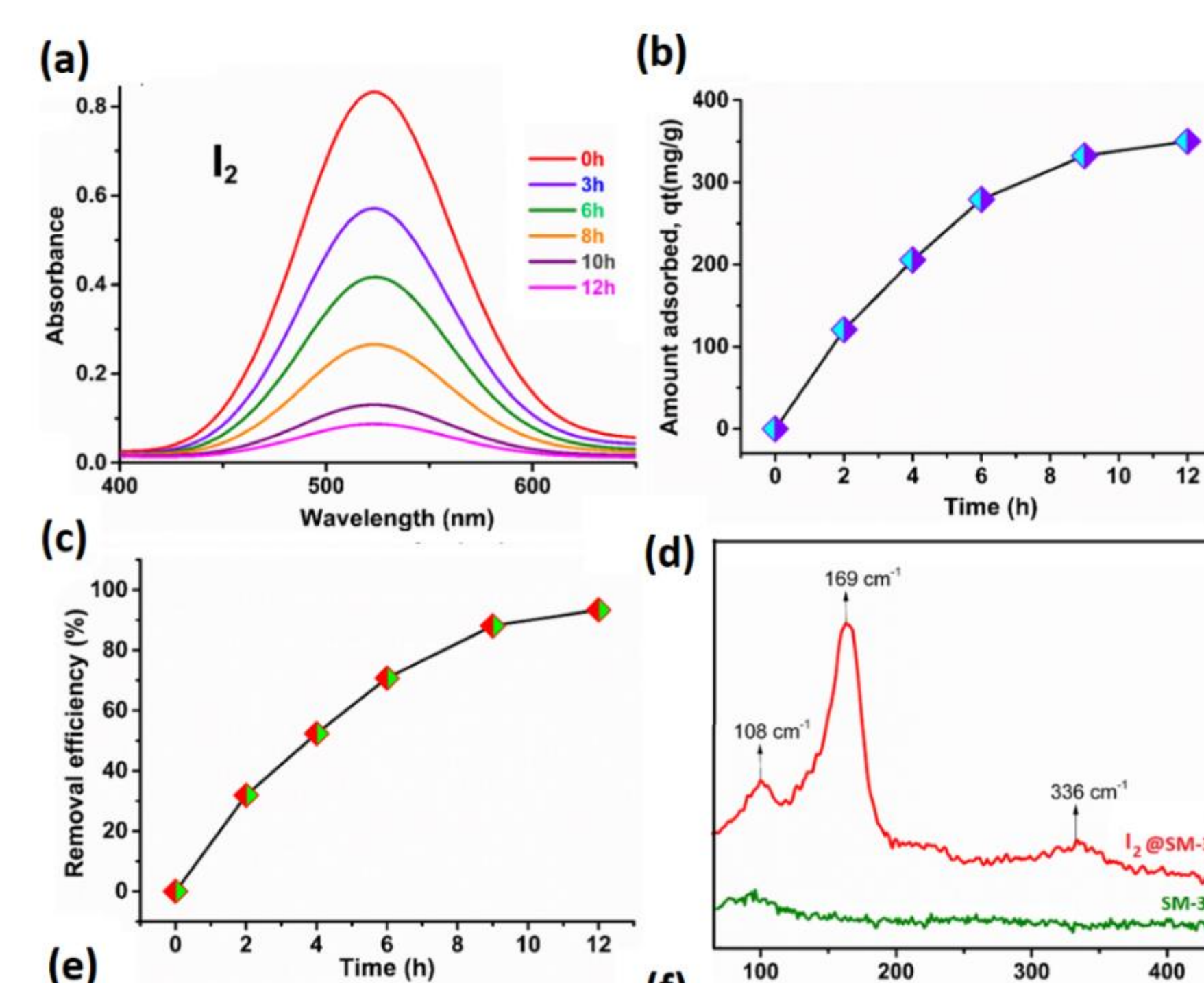


Fig. 5. UV-Vis spectra of Pb-MOF adsorbing iodine over time (b) Adsorption amounts of Pb-MOF toward iodine (c) Removal efficiency of Pb-MOF toward iodine (d) Raman spectra of SM-3 before and after iodine adsorption (e) Removal efficiency of Pb-MOF toward iodine

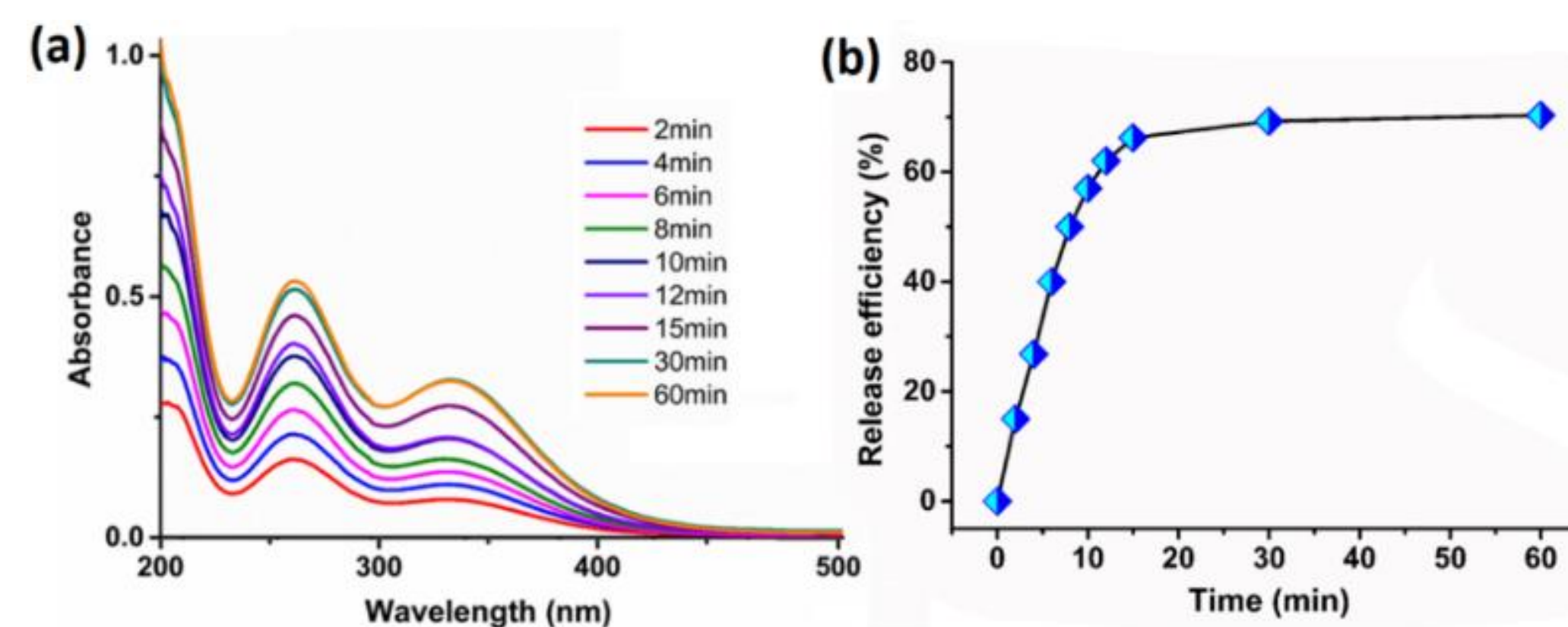


Fig. 6. (a) UV-Vis spectra for I₂ release from Pb-MOF in ethanol (b) Kinetic studies of iodine release from I₂@Pb-MOF in ethanol.

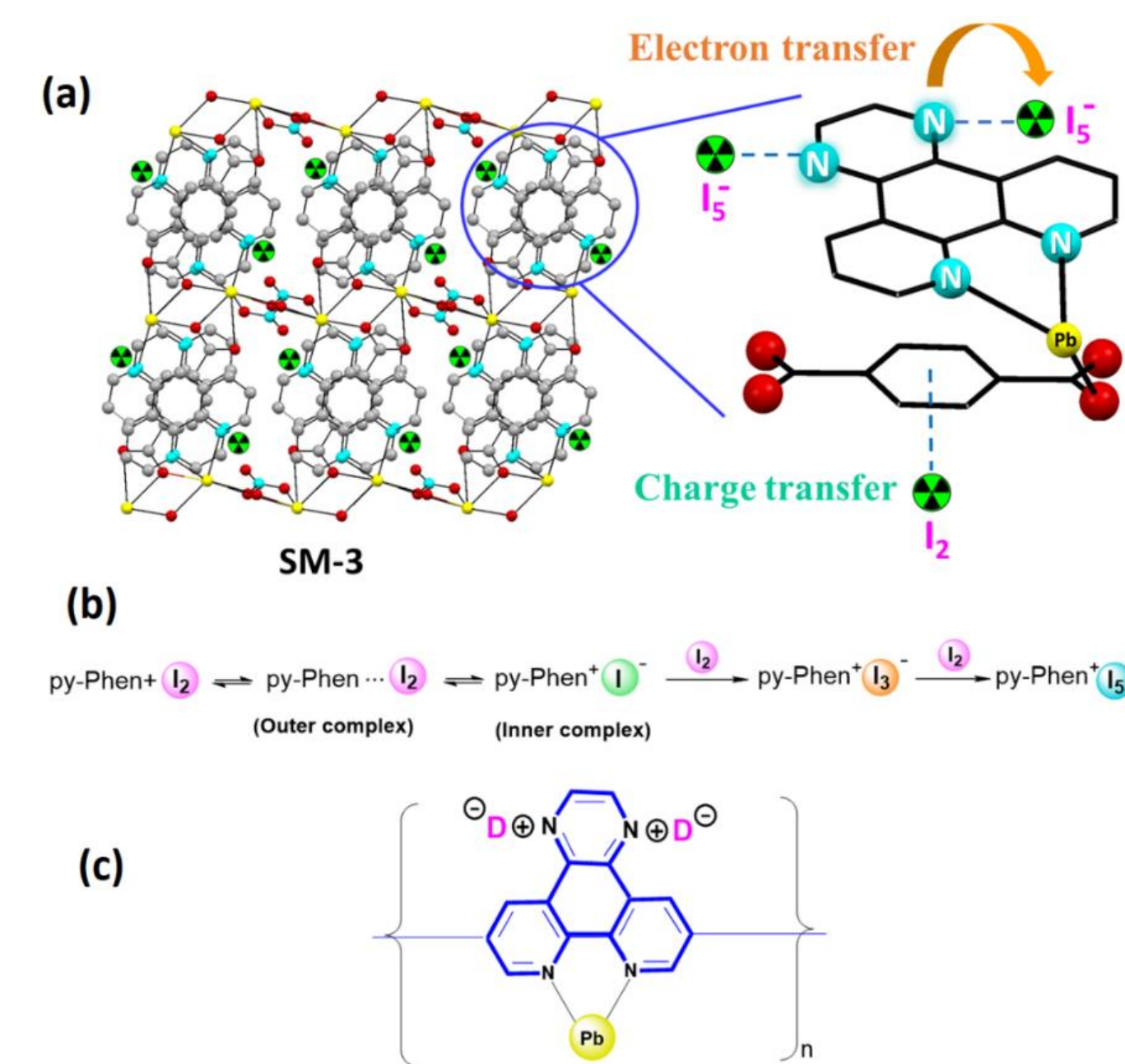


Fig. 7. Possible mechanism of iodine adsorption by Pb-MOF (b) Steps involved in the formation of polyiodide ions during iodine adsorption process, (c) structure of py-Phen'D' inner complex, where D' represents iodide (I⁻) and polyiodide (I₃⁻/I₅⁻).

6 Dye Adsorption

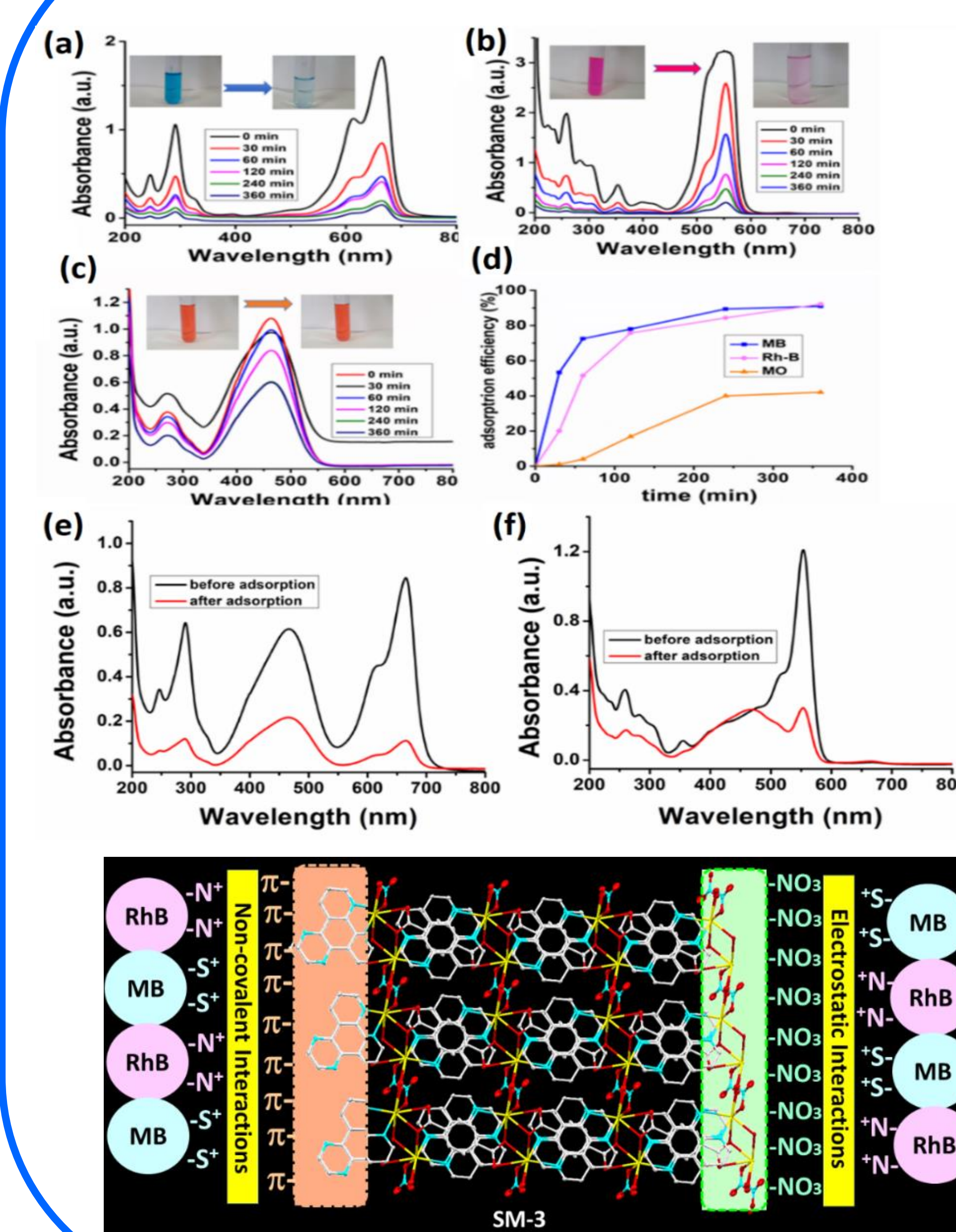


Fig. 8. Adsorption titration plots of organic dyes i.e., MB (a) Rh-B, (b) MO, (c) recorded on a UV-visible spectrophotometer using the Pb-MOF as the adsorbent, (d) Adsorption plots of MB (e) and Rh-B (f) in the presence of MO using the Pb-MOF as an adsorbent.

Fig. 9. Possible mechanism for cationic MB and Rh-B dye adsorption using MOF Pb-MOF.

Future Outlook

- This work is remarkable for coordination chemists to engineer layered MOFs for adsorption purposes and expands their potential characteristics by converting them into 2D MOF nanosheets to further enhance the adsorption of hazardous pollutants for environment protection.

Acknowledgement and References

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2. Khan, M. S., Khalid, M., Ahmad, M. S., Shahid, M., & Ahmad, M. *Dalton Trans.* 2019, 48, 12918-12932.