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#### ACCEPTED MANUSCRIPT

# Covalently Bonded Zeolitic Imidazolate Frameworks and Polymers with Enhanced Compatibility in Thin Film Nanocomposite Membranes for Gas Separation

Shuwen Yu<sup>1,2,3</sup>, Shichun Li<sup>1,\*</sup>, Shiliang Huang <sup>1</sup>, Zehua Zeng<sup>1</sup>, Sheng Cui<sup>2,3</sup>, Yu Liu<sup>1,\*</sup>

<sup>1</sup>Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, P. R.China

<sup>2</sup> College of Materials Science and Engineering, Nanjing Tech University, Nanjing 210009, P. R. China

<sup>3</sup> Jiangsu Collaborative Innovation Center for Advanced Inorganic Function Composites, Nanjing Tech University, Nanjing 210009, P. R. China

lishichun@caep.cn

liuyu307@caep.cn

\*Corresponding authors at: Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, P. R. China. Tel.: +86-816-2480534; fax: +86-816-2495856.

#### **Abstract**

Mixed matrix membranes (MMMs) for gas separation show promising applications in energy and environment related fields. However, the poor compatibility between particles and polymers in MMMs is the main problem. Zeolitic imidazolate frameworks (ZIFs) as inorganic-organic hybrid porous materials have better compatibility with polymers than other inorganic particles, but interfacial defects between ZIFs and polymers still have been observed in MMMs. In this work, the interfacial compatibility in MMMs has been enhanced by building covalent bonds between amine modified ZIF-8 (NH<sub>2</sub>-ZIF-8) and polyamide in thin film nanocomposite (TFN) membranes prepared by in situ interfacial polymerization (IP). The attendance of amino groups on the surface of NH<sub>2</sub>-ZIF-8 was confirmed by both experiments and molecular simulation. The covalent bonds formed between

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