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ZEOLITIC IMIDAZOLE FRAMEWORK MATERIALS DESIGN FOR IMPROVED ENERGY ABSORPTION PERFORMANCE

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1. Introduction *Mechanical energy dissipation, storage and conversion*







1. Introduction *MOFs for energy dissipation*









- ✓ (Super)hydrophobic materials: Contact angle >90° to enhance the Int-ext pressure
 ✓ Porous materials: Accessible pores for water intrusion and high surface areas to
- enhance the surface on int-ext takes place.
- \checkmark Tunable structure: Different chemistry, topology... \rightarrow performance optimization



Electro-Intrusion: materials for converting vibrations into electricity.



Building triboelectric nanogenerators



Project webpage: www.electro-intrusion.eu



1. Introduction *MOFs for energy dissipation*







1. Introduction *ZIF-8 as reference material*







2. H₂O intrusion mechanism

Intrusion porosimtrey and in operando synchrotron radiation





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IMMS

2024



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2. H₂O intrusion mechanism *Atomistic simulations*

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Water molecules inside each cavity (config #: 0)



3. Hybrid MOFs for energy dissipation/storage *Enhancing int-ext performance*







J. D. Sosa et al., Crystals, 2018, 8 (8), 325

- Specific design of MOFs to improve performances
- * Hot topic for usual applications: adsorption/separation, catalysis, energy storage...

LECTRO

NTRUSION

3. Hybrid MOFs for energy dissipation/storage *Bimetallic ZIF – enhancing stability*







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3. Hybrid MOFs for energy dissipation/storage *Bimetallic ZIF – enhancing stability*







* Co/Zn-ZIF present an intermediate behavior between their two parent ZIFs.

- * Hybrid ZIF combines the higher P_{int} of ZIF-8 and the higher V_{int} of ZIF-67.
- * Co/Zn-ZIF also keeps its structural integrity.

NTRUSION













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Second MOF with molecular spring behaviour (P_{int} ≈ P_{ext}).
 Previously reported zeolites with molecular spring behaviour but at much higher P → implications for applications.

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В











С

Contributions to different int-ext performance

- Effect of hydrophobicity
- Effect of flexibility
- Effect of pore size
- **Bar Effect of surface/volume ratio**
- Accomodation blm in mlm-based SOD topology implies protruding of alien linker
- Reduction of pore volume





5. Conclusions



- * Two different hybrid MOFs were tested in H_2O intrusion-extrusion experiments.
 - Bimetallic Co/Zn-ZIF combined stability and higher P_{int} of ZIF-8 and the higher V_{int} of ZIF-67.
 - ZIF-7-8 shows a non-hysteretic behavior in H₂O int-ext due to the key role of alien linker blm, affecting hydrophobicity, pore size, pore volume and surface/volume ratio.
- The possibilities offered by hybrid systems represent a new way to grant new properties or improve well-known MOFs, allowing them to maintain those characteristics essential for their dissipation performance and mechanical energy storage







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