

#### **Deliverable 4:**

Accurate description of gas adsorption, separation and storage via nanoporous materials, temperature effects, and accurate thermochemistry predictions.

<https://doi.org/10.1021/acs.jpcelett.6b02414>

<https://doi.org/10.1021/acs.jpcc.6b12959>

<https://doi.org/10.1039/C7CP05869A>

<https://doi.org/10.1039/C8CP04109A>