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High-pressure, ambient temperature hydrogen storage in metal-organic frameworks and porous carbon MATTHEW BECKNER, Optimal CAE, Inc., ANNE DAILLY, General Motors — We investigated hydrogen storage in micro-porous adsorbents at ambient temperature and pressures up to 320 bar. We measured three benchmark adsorbents: two metal-organic frameworks, Cu_3(1,3,5-benzenetricarboxylate)$_2$ [Cu_3(btc)$_2$; HKUST-1] and Zn_4O(1,3,5-benzenetribenzoate)$_2$ [Zn_4O(btb)$_2$; MOF-177], and the activated carbon MSC-30. In this talk, we focus on adsorption enthalpy calculations using a single adsorption isotherm. We use the differential form of the Claussius-Clapeyron equation applied to the Dubinin-Astakhov adsorption model to calculate adsorption enthalpies. Calculation of the adsorption enthalpy in this way gives a temperature independent enthalpy of 5-7 kJ/mol at the lowest coverage for the three materials investigated. Additionally, we discuss the assumptions and corrections that must be made when calculating adsorption isotherms at high-pressure and adsorption enthalpies.

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