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Hydrogen storage via physisorption: the combined role of adsorption enthalpy and entropy

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**Abstract:** Materials capable of cost-effective on-board hydrogen storage and delivery are currently being sought worldwide as a means to facilitate a hydrogen-based energy transition in the transportation sector. Among the solutions proposed, hydrogen storage by physisorption on porous solids constitutes a main avenue of research, and for intelligent design of such materials a detailed knowledge of gas adsorption thermodynamics is of the utmost importance. Analysis of the available data for hydrogen adsorption on alkali and alkaline-earth cation exchanged zeolites clearly shows that standard adsorption enthalpy ( $\Delta H^0$ ) and entropy ( $\Delta S^0$ ) are correlated, in the sense that larger  $\Delta S^0$  values correspond to larger  $\Delta H^0$  values. It was also shown that, referring to absolute values, the relative rate at which adsorption entropy changes decreases gradually as adsorption enthalpy increases thus resulting in a non-linear correlation between  $\Delta H^0$  and  $\Delta S^0$ . These results are discussed and corresponding implications for hydrogen storage via physisorption are highlighted.

**Key Words:** Adsorption thermodynamics; enthalpy-entropy correlation; hydrogen physisorption; hydrogen storage.

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