POROUS COORDINATION POLYMERS AND ALUMINOPHOSPHATES TRANSFORM WATER ADSORPTIVE HEAT TO DRIVE SOLAR COOLING AND HEATING

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ΠΕΡΙΛΗΨΗ

We present a recent work [1-4] on novel aluminum-based adsorbent porous materials for solar thermally driven cooling and heating processes. Such applications constitute an efficient system for adsorptive heat transformation of clean and renewable sorbates (e.g. water) within these materials. The regeneration part of the thermodynamic cycle of the system requires desorption of the sorbate at elevated temperatures, utilizing solar energy thereby minimizing primary energy consumption and carbon emissions.

The aluminium isophthalate coded as CAU-10-H is a recently synthesized porous coordination polymer (PCP) that exhibits first-rate performance for heat-pumping and cooling applications. It exhibits high uptake capacity and ability to withstand the harsh conditions imposed during repeated water sorption/desorption cycles despite its structural transition upon hydration as revealed via second-harmonic generation experiments and molecular dynamics (MD) simulations. [1]

Another newly synthesized mesoporous PCP, the aluminum benzene tricarboxylate coded as MIL-100(Al), was used for the synthesis of a bed of crystallites in order to study phase equilibria and kinetics of water sorption via pulsed field gradient (PFG) NMR experiments and MD simulations. [2] This complementary study showed that the activation energy of the intracrystalline diffusion increases upon hydration due to the progressive filling of the two interconnected pore systems in the crystal, thus verifying *a posteriori* our preceded pure simulation study in the iron MIL-100 homologue. [3]

Finally, diffusion rates of water were also investigated at temperature and loading ranges in a silico-alumino-phosphate crystal, coded as SAPO-34, bearing low silicon content, which shows reversible structural changes during water sorption/desorption cycles. [4] Similar studies were also performed for, an aluminum-phosphate coded as crystal AlPO-5 with a unidimensional microporous network. The above studies highlight the aluminum-based CAU-10-H, MIL-100, SAPO-34 and AlPO-5 among the most promising next-generation adsorbents for thermally driven cooling and heating applications.

ΒΙΒΛΙΟΓΡΑΦΙΑ

[1] Fröhlich, D.; Pantatosaki, E.; Kolokathis, P. D.; Markey, K.; Reinsch, H.; Baumgartner, M.; van der Veen, M. A.; De Vos, D. E.; Stock, N.; Papadopoulos, G. K.; Henninger S. K.; Janiak, C. (2016). *J. Mater. Chem. A,* 4: 11859-11869.

[2] Splith, T.; Pantatosaki, E.; Kolokathis, P. D.; Fröhlich D.; Zhang K.; Füldner, G.; Chmelik, C.; Jiang, J.; Henninger, S. K.; Stallmach, F.; Papadopoulos, G. K. (2017). *J. Phys. Chem. C*, 121: 18065-18074.

[3] Kolokathis P. D., Pantatosaki E., Papadopoulos G. K. (2015). *J. Phys. Chem. C,* 119 (34): 20074-20084.

[4] Stallmach, F.; Splith, T.; Chmelik, C.; Füldner, G.; Henninger, S. K.; Kolokathis, P. D.; Pantatosaki, E.; Papadopoulos, G. K. (2016). *Chemie Ingenieur Technik*, 88 (3): 372-378.