When water becomes an integral part of carbon - combining theory and experiment to understand the zeolite-like water adsorption properties of porous C_2N materials

Supporting Information

Julian Heske,[a,b] Ralf Walczak,[b] Jan D. Epping,[c] Sol Youk,[b] Sudhir K. Sahoo,[a] Markus Antonietti,[b] Thomas Kühne,[a,*] Martin Oschatz[b,d,*]

[a] Chair of Theoretical Chemistry and Center for Sustainable Systems Design, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany.

[b] Max Planck Institute of Colloids and Interfaces, Colloid Chemistry, Research Campus Golm, Am Mühlenberg 1, D-14476 Potsdam, Germany.

[c] Fakultät II: Mathematik & Naturwissenschaften, Institut für Chemie, Technische Universität Berlin, Hardenbergstr. 40, D-10623 Berlin, Germany.

[d] Friedrich-Schiller-University Jena, Institute for Technical Chemistry and Environmental Chemistry, Center for Energy and Environmental Chemistry Jena (CEEC Jena), Philosophenweg 7a, D-07743, Jena, Germany.

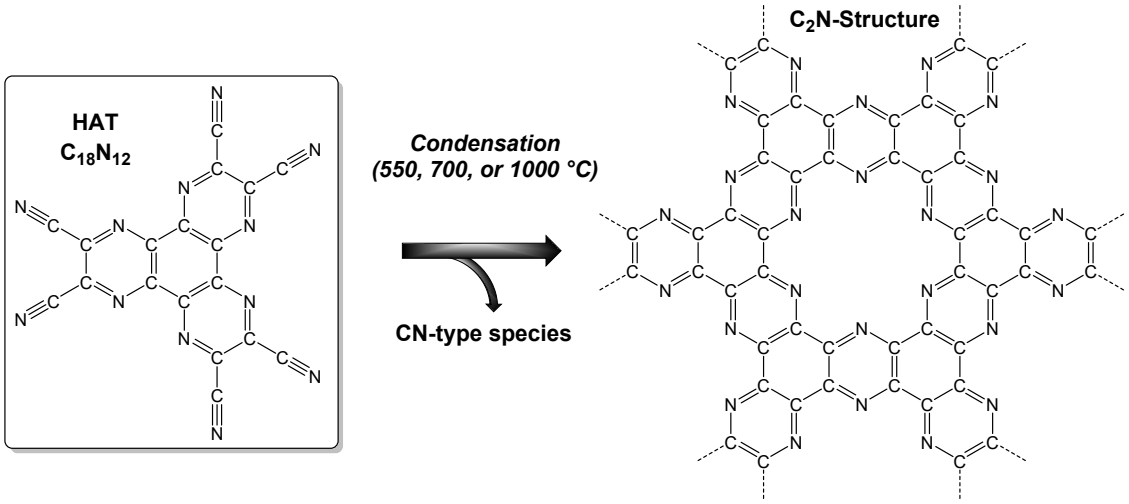

Figure S1. Thermal condensation of HAT-CN to C_2N-type products.

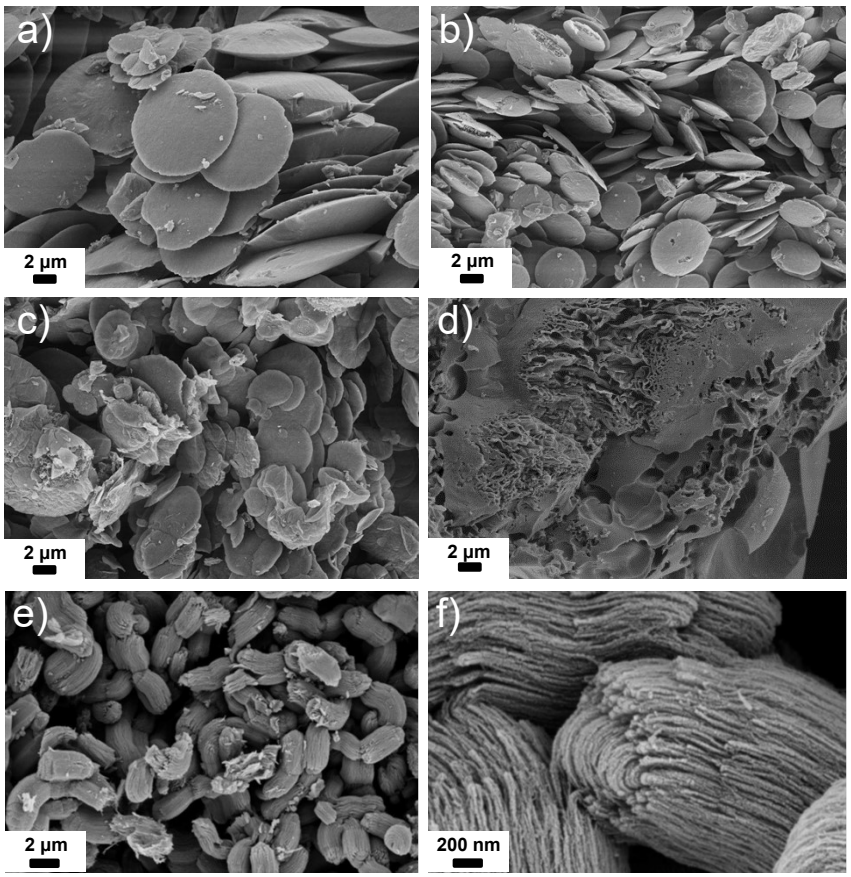

Figure S2. SEM images of C-HAT-CN-550 (a), C-HAT-CN-700 (b), C-HAT-CN-1000 (c), TiC-CDC (d), and CMK-3 (e and f).

Table S1. Adsorption energies ΔE^{ads} and incremental adsorption energies ΔE^{ads}_{inc} for different numbers of H_2O molecules adsorbed in a single pore of C_2N and C_3H, respectively.

	C_2N			**Reference C_3H**		
No. of H_2O in single interlayer	$n \cdot \Delta E^{ads}$ **[kJ/mol]**	ΔE^{ads} **[kJ/mol]**	ΔE^{ads}_{inc} **[kJ/mol]**	ΔE^{ads} **[kJ/mol]**	ΔE^{ads} **[kJ/mol]**	ΔE^{ads}_{inc} **[kJ/mol]**
1	-45.2	-45.2	-45.2	-32.8	-32.8	-32.8
2	-88.6	-44.3	-43.5	-64.2	-32.1	-31.4
3	-133.2	-44.4	-44.6	-95.6	-31.9	-31.4
4	-191.1	-47.8	-57.9	-124.7	-31.2	-29.1
5	-149.3	-29.9	+41.7	+690.8	+138.2	+815.5
4 in each interlayer	-758.0	-47.4		-504.2	-31.5	

Atomic coordinates of the final adsorption state (four adsorbed molecules in each pore) of water in C_2N as well as in the reference system are available for download at: https://doi.org/10.5281/zenodo.4469324.