Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

Zeolite framework functionalisation by tuneable incorporation of various metals into the IPC-2 zeolite

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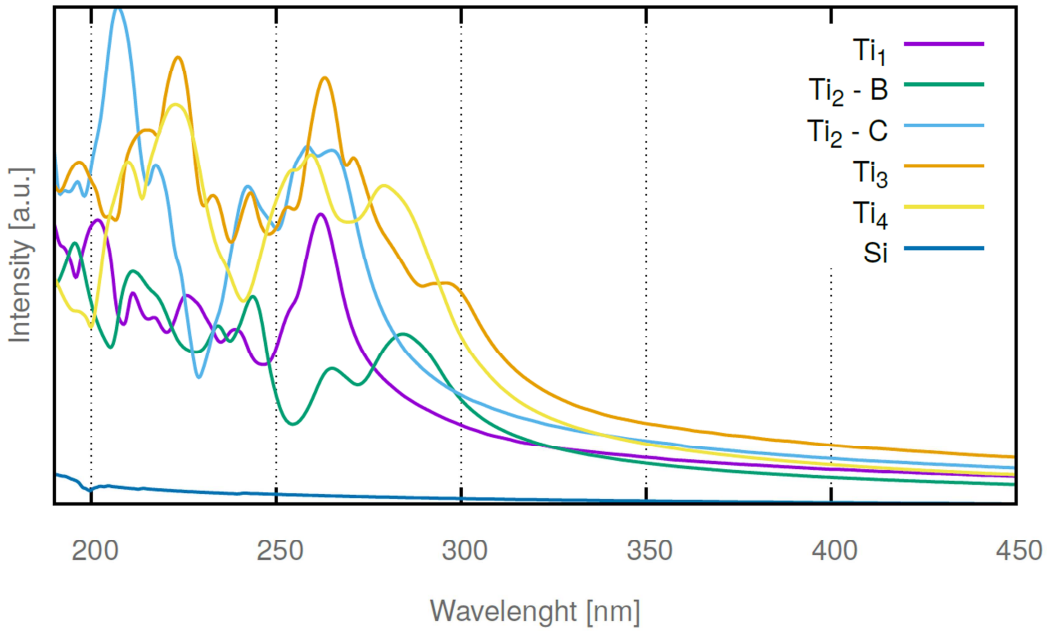

Figure ESI1. Optical properties of Ti-IPC-2 materials with Ti atoms located in the s4r units and Si-IPC-2 zeolite. Ti_1 – one atom per s4r, Ti_2 – two atoms per s4r unit (B – next to each other, C – in the opposite positions in s4r), Ti_3 – three atoms per s4r unit, Ti_4 – four atoms per s4r unit.

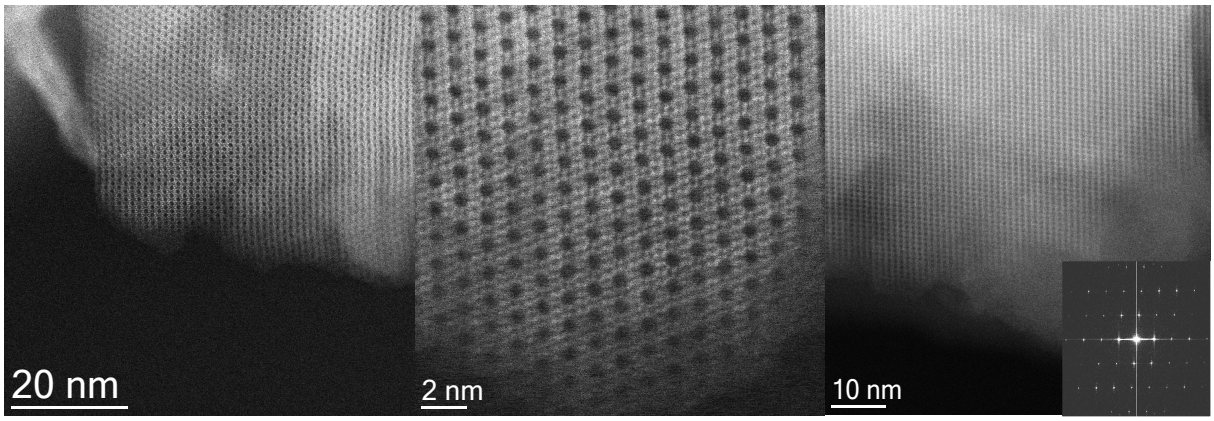

Figure ESI2. STEM micrographs of Zr-IPC-2 zeolite: view at 001 plane (left), view at 010 plane (middle), and view at 100 plane (right).

Computational methods

The computational analysis was completed using the software VASP [1], the Projected-Augmented wave function (PAW) method [2] and the pseudopotential. All structures were fully optimized using the PBEsol functional [3] to reduce the forces below 0.01 eV/Å constraining the eventual space group. After careful convergence of the parameters, we considered only gamma-point calculations with a plane wave cut-off of 700 eV. The electronic convergence was set to 10^{-6} eV.
The optical properties were calculated using the Vaspkit software [5] from the frequency dependent dielectric matrix, which was obtained accordingly to ref. [4], as implemented in VASP, increasing the number of electronic bands. In the case of aluminium, we balanced the charge of the system with a mean background charge.

References:
[1] Kresse, G., Phys. Rev. B 54.11 (1996): 169.
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[3] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, and K. Burke, Phys. Rev. Lett. 100, 136406 (2008).
[4] M. Gajdoš, K. Hummer, G. Kresse, J. Furthmüller, F. Bechstedt, Phys. Rev. B 73, 045112 (2006).
[5] https://sourceforge.net/projects/vaspkit/