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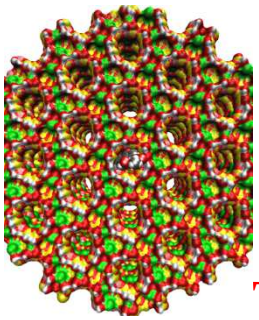
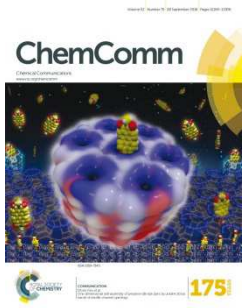


Through zeolite pore entrances



One-Dimensional Self-Assembly of Perylene-Diimide Dyes by Unidirectional Transit of Zeolite Channel Openings

http://dx.doi.org/10.1039/c6cc05303c

See also the movie: http://www.rsc.org/suppdata/c6/cc/c6cc05303c/c6cc05303c2.mp4

What's it about?

How can a snake swallow a mouse bigger than its mouth? Weird as it seems, questions like this emerge very often at the molecular scale. For example, we can fill porous materials with molecules larger than the diameter of the pores: in this way, we may obtain devices for energy and health applications.
What makes this useful process possible? Flexibility is the key: both the porous host (the "snake") and the molecule (the "mouse") must deform for the uptake to occur. But here, contrary to the mouse-snake case, cooperation between the two partners is also needed.

Why is it important?

- For the first time we captured the slipping of a bulky molecule through a narrow opening. We did this by computer simulations, because it is very hard to get information experimentally.
- We noticed that the channel opening resembles a funnel: it is larger at the entrance. This surely helps the molecule to go in.
- Also, we have seen that the molecule is drawn to the entrance by host-guest dependent intermolecular forces.
- However, the molecule can pass through the entrance and slip inside the pore only because it's flexible, and its motion is "in tune" with the vibrations of the host matrix.
- All this factors cope to make the entrance process more favorable than the exit process - that's why the molecule gets finally swallowed by the pore.

Perspectives

We've found out how bulky molecules may cross the narrow entrances of a porous host, and understood why these molecules actually prefer to enter the channels. This explains why the hybrid composite forms and remains stable. In perspective, this knowledge might help to improve the fabrication processes of a class of materials with strategic applications.