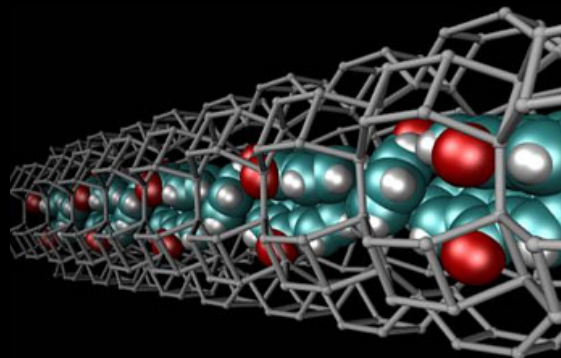


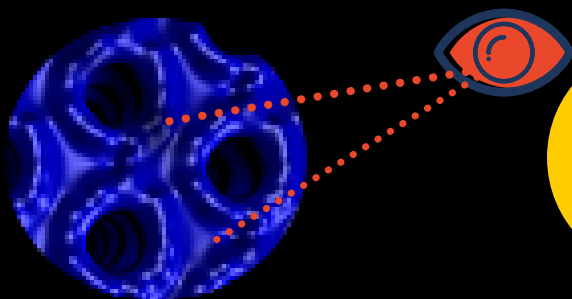
plugging the entrance of a zeolite nanochannel

Know the facts

Zeolites are porous solids used as molecular sieves, catalysts and nano-containers. Their channel entrances - fundamental for these applications - are little known at the molecular scale, and difficult to study experimentally.



STEP
01



STEP
02

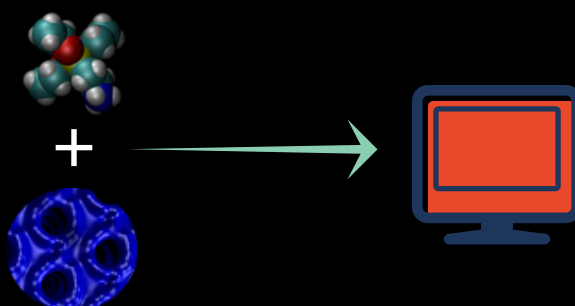
Study the bare entrance

Set up a computational model of the channel entrance and calculate its most stable structure

Modify the entrance with a molecular stopper

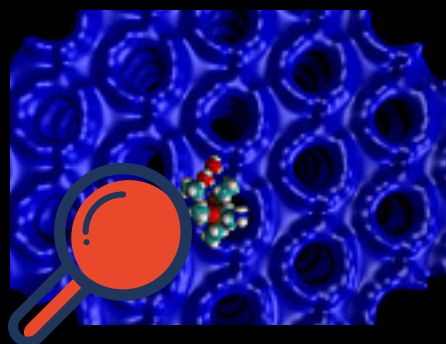
Different stopper molecules are attached to the channel entrance. The optimal geometry of the models with modified channel entrances is calculated.

STEP
03



Watch the effect of the stopper

The microscopic structure of modified channel entrances is now unraveled: a stopper may behave like a lid or a cork according to its shape, size and type. Done! Time to party and celebrate!



STEP
04

See why it's important

Now that we better know the entrances of porous host matrices, it will be easier to modify them in laboratory to create novel and useful materials.

STEP
05

