Structure Determination of Zeolite Nanosheets
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Zeolites:
- ordered micropores of molecular size
- Gas separation using zeolite membranes: an approach that can significantly save energy in chemical production.

**The importance of zeolite nanosheets**

Smaller seeds: thinner membranes, less defects, and higher flux.

**Dispersible zeolite nanosheets:**
- The smallest building unit (unit-cell-thick) for zeolite membranes.

**Car-Parrinello Molecular Dynamics**
- QuantumESPRESSO
- Covalent system
- Ground-state electronic properties
- Parallel computing is needed because of the large size of zeolite unit cells.
- Example: MFI - 1.5 unit cells

**Transmission Electron Microscopy**
- MFI (b-axis)
- MWW (c-axis)

**Powder X-Ray Diffraction**
- 1.5 unit cell MFI
- 1 unit cell MWW

**Spectroscopy**
- The fraction of surface Si atoms of the 1.5 unit cell model agrees with solid-state NMR experiment.

**Structure Determination Strategy**
- Structure determination was performed using AFM (atomic force microscopy), XRD (X-ray diffraction), TEM (transmission electron microscopy), and solid-state NMR, by comparing experiments results with simulations from the proposed models.
- Obtaining a realistic and relaxed surface structure is the first step for the simulations.

**Proposed Structural Models**
- MFI - 1 unit cell thick (1.99 nm)
- MFI - 1.5 unit cells thick (3.21 nm)
- MWW - 1 unit cell thick (2.49 nm)

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