Combining computational and experimental studies for a better understanding of cellulose and its analogs

Description

A must-read review article, where the author draws his perspective of how computational efforts should be combined with well-designed experiments to be directly compared with molecular modeling.

- **Introduction**
- **From primitive models to atomistic details**
- **Toward experimental structures with higher precision**
- The limit of experimental determination
- Limitation in resolution
- Inherent structural disorder and dynamics
- **Modeling crystals and prediction of experimental response**
- Force-field modeling and first-principles calculations
- Simulation of wave scattering
- Molecular vibration
- Nuclear magnetic resonance
- Elastic tensors
- Understanding the underlying interactions and thermodynamics
- **Conclusions**
  References

Category

1. News