Ab initio proton conduction in self-assembled aggregates of phosphonated hexaphenylbenzene

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In the scope of this project, we will perform ab-initio molecular dynamics simulations to examine and understand the microscopic processes which govern proton conduction in modern fuel cell membrane materials. In particular, we focus on phosphonated hexaphenylbenzene(p-6PA-HPB), an organic compound which has the ability to self-assemble to columnar stacks. This arrangement is very peculiar and may provide a structural base for directed proton conduction along the stack axis. In contrast to many standard materials, this material does not rely on quasi-liquid water for proton conduction, but instead is able to sustain long-range proton transport under non-humid environmental conditions.

From the fundamental theoretical side, the specific characteristics of the proton transport mechanism are also of very high relevance: In a related material, we could recently show that two commonly assumed mechanistic principles (Grotthuss and vehicle mechanisms) are actually co-acting in a combined fashion.

Our simulations will eventually lead to improved membrane materials for fuel cell applications, and hence foster the transition from our present fossile fuel based economy towards a renewable energy system.

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