

**Supporting Information:**  
**Molecular Insights into the Water Dissociation and Proton  
Dynamics at the  $\beta$ -TaON (100)/Water Interface**

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## S1. Input Files for Simulation

The CPMD input files and the coordinate file (in XYZ format) for modeling the  $\beta$ -TaON (100)/Water interface are available via the GitHub Repository at [https://github.com/mandal13/TaON\\_100\\_Water](https://github.com/mandal13/TaON_100_Water).