Dr. Tamar Stein

Fritz Haber Research Center for Molecular Dynamics

Department of Chemistry

The Hebrew University of Jerusalem

Givaat Ram 9190401, Israel

tamar.stein@mail.huji.ac.il

Dr. Nathalie Weickgenannt and Dr. Frank Maaß

Executive Editors

*Angewandte Chemie*

May 29, 2022

Dear Dr. Nathalie Weickgenannt and Dr. Frank Maaß:

I am pleased to submit an original research article entitled “Squeezing Water Clusters within Anthracene Dimers” by Drs. Molina, Xu, Kostko, Ahmed, and myself for consideration for publication in *Angewandte Chemie.*

This manuscript studied anthracene monomers and dimers with water-cluster systems utilizing molecular beam vacuum-UV photoionization mass spectrometry and density functional calculations. Our calculations revealed that the energetic tendency of water was to remain clustered around the polycylic aromatic hydrocarbons (PAHs), rather than disperse. We report the optimal molecular-level conditions that are essential for water confinement inside PAHs, which is crucial in various applications. We observed water confinement exclusively in the case of four-water clusters and only when the anthracenes were in a cross configuration due to optimal OH⋯π interactions, indicating dependence on the size and structure of the PAH. Structural changes in the water occurred upon ionization of the anthracene, guided by the optimal interactions of the resulting hole and water hydrogen atoms. Structural loss in the photoionization efficiency curves when adding water indicated that various isomers were generated, while theory suggested only a slight shift in energy in photoionization states of different isomers.

We believe that this manuscript is appropriate for publication in *Angewandte Chemie* because the the journal aims to increase knowledge and understanding in chemical research across all fields of chemistry and adjacent disciplines.

This manuscript has not been published before and is not under consideration for publication elsewhere.

Thank you for your consideration!

Sincerely,

Dr. Tamar Stein

Fritz Haber Research Center for Molecular Dynamics

Department of Chemistry

The Hebrew University of Jerusalem