

ABSTRACT

Competition among hydrogen and chalcogen bonds in interactions between chalcogen hydrides

Sotiris Xantheas

Department of Chemistry, University of Washington, Seattle, WA 98195, USA
Advanced Computing, Mathematics and Data Division, Pacific Northwest National Laboratory,
902 Battelle Boulevard, P.O. Box 999, MS J7-10, Richland, WA 99352, USA
Computational and Theoretical Chemistry Institute (CTCI), Pacific Northwest National
Laboratory, Richland, WA 99352, USA

Hydrogen bonds are fundamental in determining the macroscopic properties of water (H₂O) that are distinctively different (“anomalously high” melting, boiling and critical points, maximum density at 4° C etc.) from those of the hydrides of the rest of the chalcogens (H₂S, H₂Se, H₂Te). While water molecules interact solely via hydrogen bonds, the hydrides of the rest of the chalcogens (S, Se, Te) can interact via either hydrogen or chalcogen bonds. The properties of these new bonds that govern the interactions in hydride of the heavier elements of group 16 of the periodic table have been probed via the analysis of the wavefunctions and the components of the total interaction. In addition, the analysis of the vibrational infrared spectra of these bonds reveals specific spectral signatures that can be used for their experimental identification. The molecular picture that emerges from the analysis of the fundamental interactions between hydrogen bonds suggests a quantitative relationship between energy – structure – spectroscopy that can be used for the assignment of the experimental spectra and their use in determining the bond structure at the molecular level.

MP Hoffman and SS Xantheas, *Journal of the American Chemical Society* **147**, 11152-11171 (2025).

MP Hoffman and SS Xantheas, Michael Duncan Festschrift, *Journal of Physical Chemistry A* in press (2025); <https://doi.org/10.1021/acs.jpca.5c06655>

MP Hoffman and SS Xantheas, *Journal of the American Chemical Society* under review (2025).

KM Herman and SS Xantheas, *Journal of the American Chemical Society* **147**, 29732 (2025).

MA Boyer, O Marsalek, JP Heindel, TE Markland, AB McCoy, and SS Xantheas, *Journal of Physical Chemistry Letters* **10**, 918 (2019).

GD Santis and SS Xantheas, *Journal of Chemical Physics* **162**, 044106 (2025).

GD Santis and SS Xantheas, *Journal of Chemical Physics* **162**, 244121 (2025).

GD Santis and SS Xantheas, Mark A. Johnson Festschrift, *Journal of Physical Chemistry A* **129**, 9930 (2025).