Invited Lecture

H_2O ices in the Solar System

C. G. Salzmann,[1] A. Amon,[1] S. T. Bramwell,[1] C. L. Bull,[2] B. Chikani,[1] M. B. Davies,[1,3] M. G. Fox-Powell,[4] H. Fraser,[4] S. O. Halukeerthi,[1] R. E. Hamp,[4] M. Hart,[1] P. Harvey,[1] T. F. Headen,[2] A. Michaelides,[3] B. J. Murray,[5] L. C. Pardo,[6] A. Rosu-Finsen,[1] A. Sella,[1] Z. Sharif,[1] J. J. Shephard,[1] B. Slater,[1] S. K. Talewar,[1] H. Wu[1]

[1]University College London, London WC1H 0AJ, UK, [2] ISIS Pulsed Neutron and Muon Source, Didcot OX11 0QX, UK, [3]University of Cambridge, Cambridge CB2 1EW, UK, [4]The Open University, Milton Keynes MK7 6AA, UK, [5]University of Leeds, Leeds LS2 9JT, UK, [6]Universitat Politècnica de Catalunya, E-08019 Barcelona, Spain
c.salzmann@ucl.ac.uk

Water (H_2O) is the third most abundant molecule in the Universe following dihydrogen and carbon monoxide. Travelling through the Solar System, water ice is a constant companion from the polar regions on Earth and the asteroid belt to the icy satellites of the gas giants and the Kuiper belt. The presence of ice across the Solar System is important for a variety of reasons: Firstly, ice can transform to liquid water which is the key component for the search for extra-terrestrial life. Secondly, the properties and phase transitions of the many different types of ice may influence atmospheric and geological processes. Finally, the presence of ice outside of Earth is an important technological factor for space exploration in terms of the creation of rocket fuel and water supply for crewed missions. In this talk, we will discuss our recent work on the various crystalline and amorphous forms of ice, and their relevance with respect to geological and atmospheric processes in the Solar System.

High-pressure phases of ice are expected to occur in the thick ice shells of the ice moons of the gas giants. The presence of salts can alter their phase stabilities and in one case, using ammonium fluoride as a dopant, the ice II high-pressure phase of ice was even selectively removed from the phase diagram as demonstrated by in-situ pressure neutron diffraction [1,2]. Up until recently, the 'ordinary' ice I was thought to exist in either the stable hexagonal (ice I*h*) or the metastable cubic form (ice I*c*). We discuss that the occurrence of ice I*c* in the Solar System is unlikely and that metastable ice I is expected to exist as stacking disordered ice (I *sd*) which consists of variable amounts of hexagonal and cubic stacking.[3] Fig. 1 shows locations in the Solar System where the presence of ice I*sd* is possible. In diffraction, the stacking disorder results in asymmetric broadening of some of the Bragg peaks which we fit with our MCDIFFaX program. Depending on the parent material and thermal history of ice I*sd* samples, different characteristics of the stacking disorder are found which offers the exciting prospect of using stacking disorder as a marker for the geological history of ice I samples [3].

Cryogenic ball-milling of ice I*h* has recently led to the discovery of medium-density amorphous ice which may be present in some of the ice moons as a consequence of tidal forces [4]. Finally, mixtures of low-density amorphous ice and hydrophobic hydrocarbons were prepared as the exist in comets [5]. The effects of the hydrocarbons on the crystallisation temperature and H_2O desorption properties were investigated, and the structure of water in the first hydration shell of adamantane ($C_{10}H_{16}$) was solved with neutron diffraction.

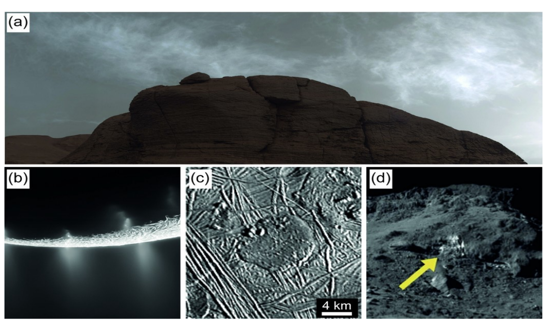

Figure 1. Potential occurrences of ice I*sd* in the Solar System.[3] (a) Clouds on Mars. (b) Plumes of vapour and ice at Enceladus. (c) A 'dome'; a quasi-circular feature in Europa's Conamara region. (d) A high-albedo patch on comet 67P/Churyumov-Gerasimenko.

[1] Shephard, J. J., Slater, B., Harvey, P., Hart, M., Bull, C. L., Bramwell, S. T, Salzmann, C. G. (2018) *Nat. Phys.*, **14**, 569.

[2] Sharif, Z., Slater, B., Bull, C. L., Hart, M. & Salzmann, C. G. (2021) *J. Chem. Phys.*, **154**, 114502.

[3] Salzmann, C. G., Murray, B. J., Fox-Powell, M. G., Hamp, R. E., Rosu-Finsen, A. & Fraser, H. (2024) *Icarus*, **410**, 115897.

[4] Rosu-Finsen, A., Davies, M. B., Amon, A., Wu, H., Sella, A., Michaelides, A. & Salzmann, C. G. (2023) *Science*, **379**, 474.

[5] Talewar, S. K., Pardo, L. C., Headen, T. F., Halukeerthi, S. O., Chikani, B., Rosu-Finsen, A. & Salzmann, C. G. (2024) Faraday Discuss.,**249**, 69.