Pressure response of Prussian white - multidimensional phase diagram of an important cathode material

Elina Elvelo,[1,2] Dominik Daisenberger[3], Nicholas P.Funnell[4], Craig L. Bull[4], Andrew B. Cairns[2], Hanna L. B. Boström[1]

1 Department of Chemistry, Stockholm University; 2 Department of Materials, Imperial Collage of London; 3 Diamond Light Source; 4 ISIS Neutron and Muon Source

elina.elvelo@su.se

Development of new batteries is an ever-relevant topic for industry as well as society at large. There is a need for more sustainable batteries, sodium ion batteries are promising candidates and Prussian white (PW) is a potential cathode material. [1]

PW, $Na_2FeFe(CN)_6 \cdot n\ H_2O$ is a Prussian blue analogue (PBA), a class of materials of transition metal-cyanide networks with a hidden world of structural complexity. The thermal phase behaviour of PW is well known [1, 2], but the pressure response has not been investigated. A pressure study would elucidate the effects of interstitial water, as hydration is decoupled from pressure, unlike heating which leads to dehydration.

This project utilises high-pressure X-ray and neutron powder diffraction to study the structure of hydrated PW expanding the existing phase diagram to regard temperature and pressure but also on sodium- and water-content. A rich phase behaviour is unveiled, with new identified phases including a possible low spin configuration on both iron sites [3].

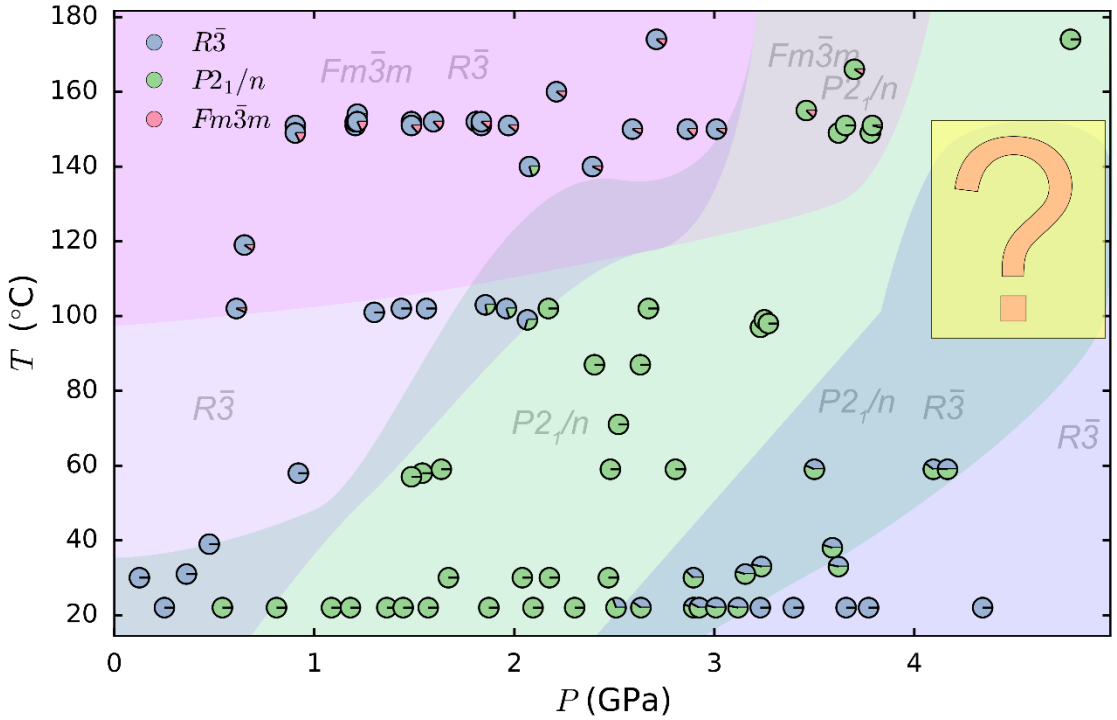


Figure 1. *Preliminary pressure-temperature phase-diagram of hydrated PW from variable pressure, variable temperature X-ray data. The yellow area highlights the uncertain region with the unknown superstructure.*

[1] I. Nielsen et al, J. Phys. Energy. (2022). 4, 044012
[2] H. Tokoro and S.-I. Ohkoshi, Dalton Trans. (2011). 40, 6825–6833.
[3] H. L. B. Boström, A. B. Cairns, L. Liu, P. Lazor, I. E. Collings, Dalton Trans. (2020). 49, 12940–12944

Acknowledgments: Wallenberg Initiative Material Science for Sustainability.