

# Statistical mechanics models for the PdH<sub>x</sub> and PdD<sub>x</sub> phase diagram with both O-site and T-site occupation

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In past years we developed statistical mechanics models for bulk PdH<sub>x</sub> separately for the alpha phase [1] and for the beta phase [2], and also to model the isotherms of the phase diagram [3]. We recently extended this analysis to develop a similar model for the phase diagram of PdD<sub>x</sub>.

One issue encountered concerns the data sets available for PdD<sub>x</sub>. For PdH<sub>x</sub> it was possible to make use of previous work that was put into the development of a phase diagram based on individual isotherm measurements. There do not appear in the literature analogous phase diagrams constructed for PdD<sub>x</sub>.

A second issue encountered concerns extrapolation into regions of higher loading. For PdH<sub>x</sub> it was possible to make use of experimental data at relatively high loading and high temperature to develop plausible extrapolations. However, there are fewer available data sets for PdD<sub>x</sub>, and these do not permit an analogous extrapolation.

- [1] P. L. Hagelstein, "Empirical models for octahedral and tetrahedral occupation in PdH and PdD at high loading," J. Condensed Matter Nuclear Science, vol. 17, pp. 35-66, 2015.
- [2] P. L. Hagelstein, "O-site and T-site occupation of  $\alpha$ -phase PdH<sub>x</sub> and PdD<sub>x</sub>," J. Condensed Matter Nuclear Science, vol. 17, pp. 67-90, 2015.
- [3] P. L. Hagelstein, "Models for the phase diagram of palladium hydride including O-site and T-site occupation," J. Condensed Matter Nuclear Science, vol. 20, pp. 54-80, 2016.