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Palladium (II) in Liquid Ammonia : An Investigation of Structural and Dynamical Properties by applying Quantum Mechanical Charge Field Molecular Dynamics (QMCF–MD) – Supplementary Material

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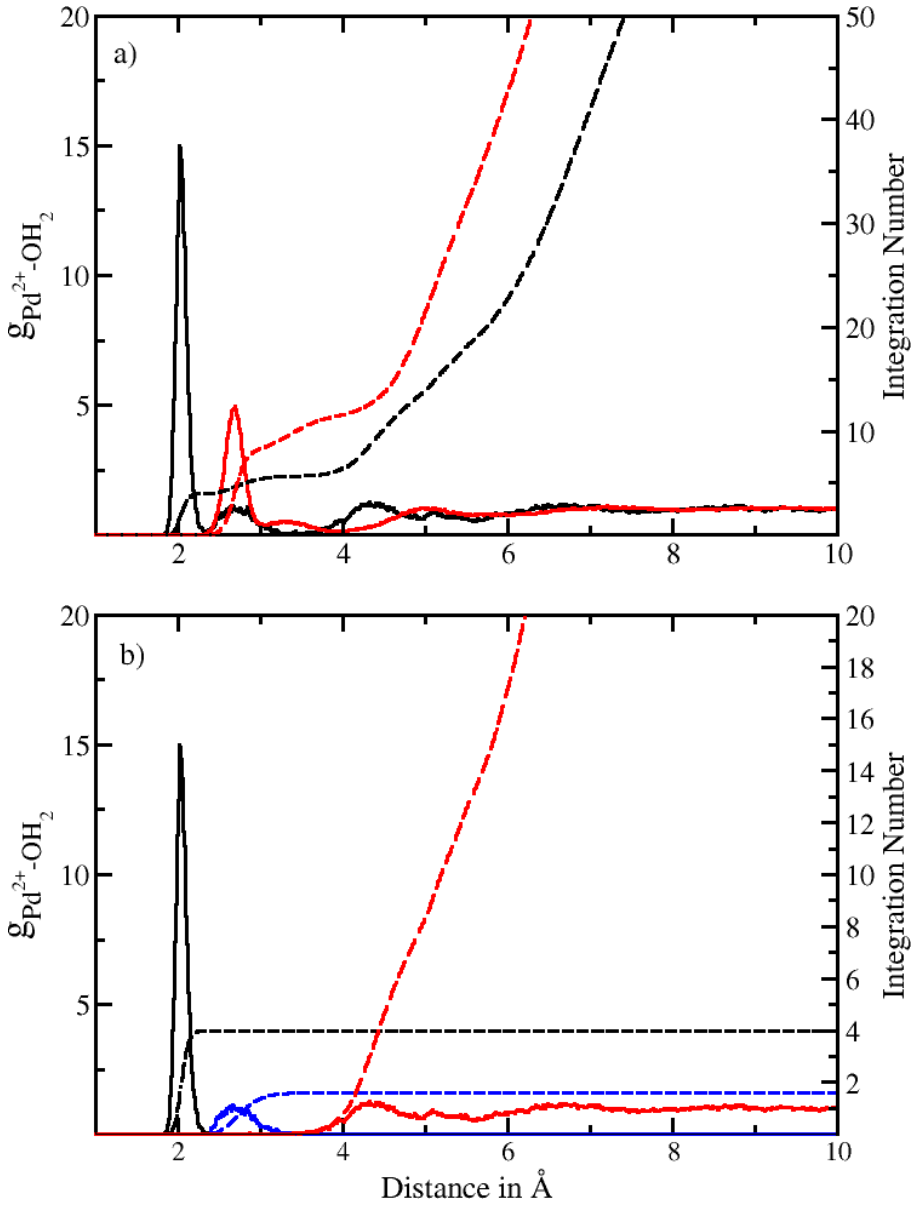

Figure S1: a) Pd^{2+}-O (black solid) and Pd^{2+}-H (red solid) radial distribution functions (RDFs) and their integration number (dash line) obtained via a previous QMCF-MD simulation.[1] b) Decomposition of the Pd-O RDF according to a combined angular-radial criterion showing the first shell (solid black), extended first shell (solid blue) and second shell plus bulk (red solid) and the associated running integration numbers (dashed).

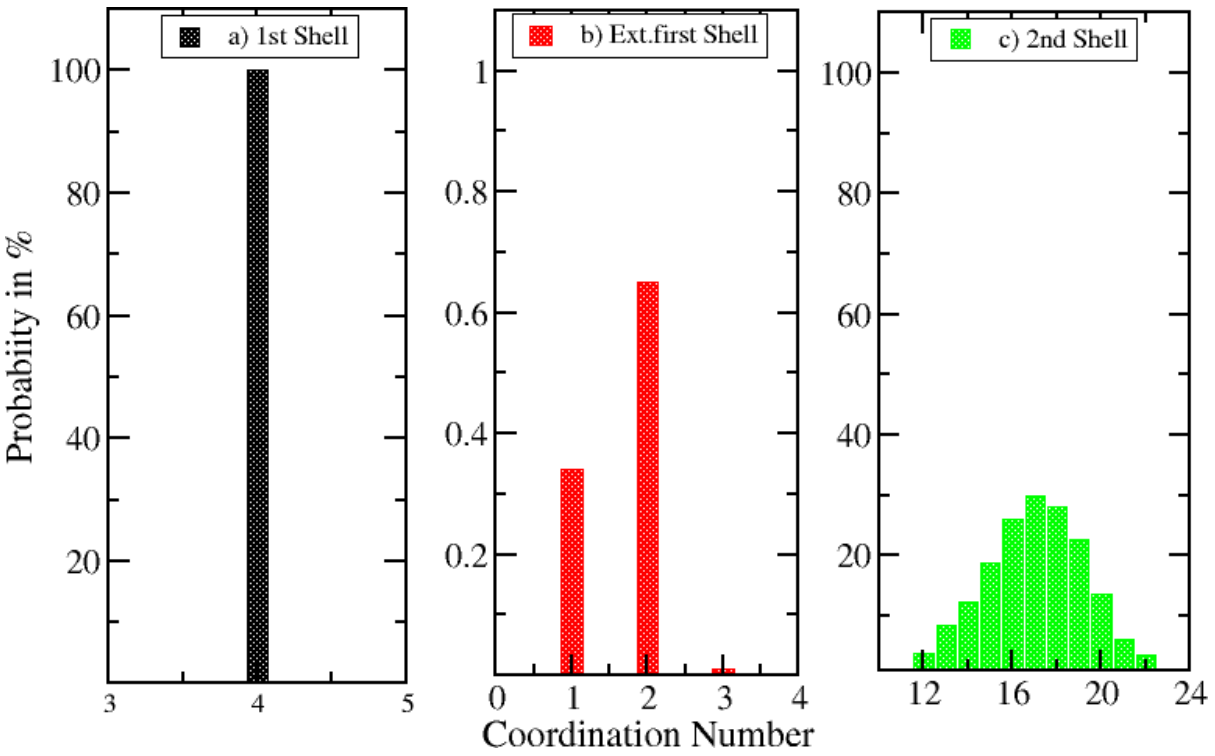

Figure S2: Coordination number distributions (CNDs) of the first, ext. first and second solvation shells of Pd^{2+} in aqueous solution obtained from a previous QMCF-MD simulation.[1]

References

[1] T. S. Hofer, B. R. Randolf, S. A. A. Shah, B. M. Rode, and I. Persson, *Chem. Phys. Lett.*, 2007, **445**(4), 193–197.