

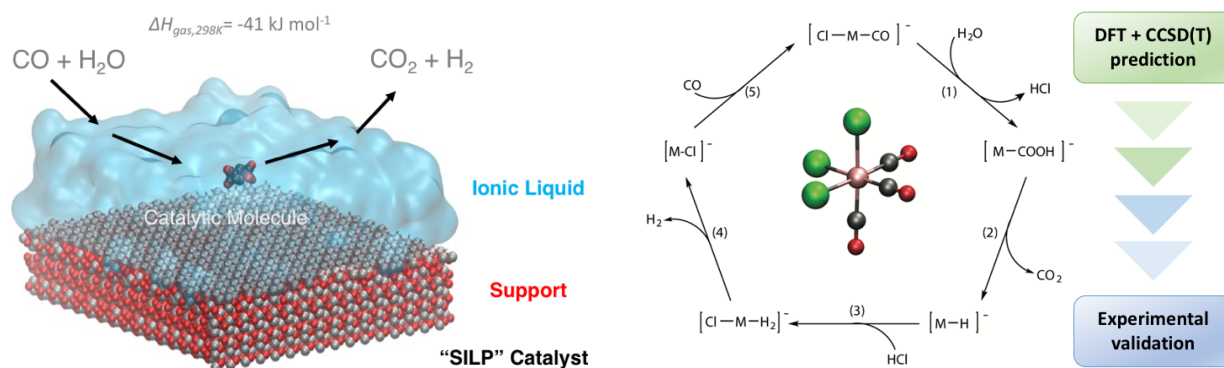
# Modelling SILP Catalysis: The Water-Gas-Shift Reaction

R. Stepić,<sup>1</sup> C. R. Wick,<sup>1,2</sup> N. Vučemilović-Alagić,<sup>1,3</sup> D. M. Smith,<sup>1,3</sup> A.-S. Smith<sup>1,3</sup>

<sup>1</sup>PULS Group, Institute of Theoretical Physics, FAU Erlangen-Nürnberg, Germany

<sup>2</sup>Zentralinstitut für Scientific Computing (ZISC), FAU Erlangen-Nürnberg, Germany

<sup>3</sup>Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia



Supported ionic liquid phase (SILP) catalysts facilitate a highly efficient, homogeneously catalyzed water-gas shift reaction (WGS) at ultra-low temperatures between 120 °C and 150 °C. [1,2] SILP catalysts consist of an ionic liquid (IL) covering a porous support, while the actual catalytic molecule is dissolved in the IL phase. Thus, the SILP catalysts allow fine tuning of the actual catalytic reaction as well as the reaction conditions *via* variation of the support, the IL, the molecular catalysts and addition of additives.

Ru-based transition metal complexes have been identified as one of the most promising molecular catalysts in SILP conditions for the water-gas shift reaction (WGS). The active Ru-complexes have been found to exist in imidazolium chloride melts under operating conditions in a dynamic equilibrium, which is dominated by the [Ru(CO)<sub>3</sub>Cl<sub>3</sub>]<sup>-</sup> complex.[3] A detailed theoretical and experimental investigation showed that the reaction mechanism for this type of catalytic species includes the intermediate formation and degradation of hydrogen chloride, which effectively reduces the high barrier for the formation of the requisite dihydrogen complex. The hypothesis that the rate-limiting step involves water is supported by using D<sub>2</sub>O in continuous catalytic WGS experiments. [4]

In addition to the elucidation of the reaction mechanism in SILP catalysis, we investigated the effect of CuCl additives with respect to the WGS reaction. Again, density functional theory (DFT) calculations and in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) measurements have been used to identify the role of CuCl as CO shuttle, which leads to an enhancement of the catalytic performance. [5,6]

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