Recent Advances in Py-ChemShell's Development for Modelling Hetero- and Homogeneous Catalysis

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ChemShell, one of the most popular computational chemistry environments for multiscale simulations [1,2], has been widely used for modelling hetero- and homogeneous catalysis [3], especially using the QM/MM approaches. This presentation will showcase the most recently developed features in the new Python-based ChemShell (i.e. Py-ChemShell) that will greatly facilitate simulations for the community. Highlights include: support for QM/MM models with ghost atoms of vacancy-defective metal oxides, a guided workflow for automated solvation of a molecule/cluster and setup of QM/MM model, a generic inbuilt MD driver driven by DL_POLY 5, and so on.

Acknowledgments
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[1] Y. Lu, et al., "Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment", J. Chem. Theory Comput., 15, 1317-1328 (2019)
[2] www.chemshell.org
[3] Y. Lu, et al., "Multiscale QM/MM modelling of catalytic systems with ChemShell", Phys. Chem. Chem. Phys., 25, 21816-21835 (2023)

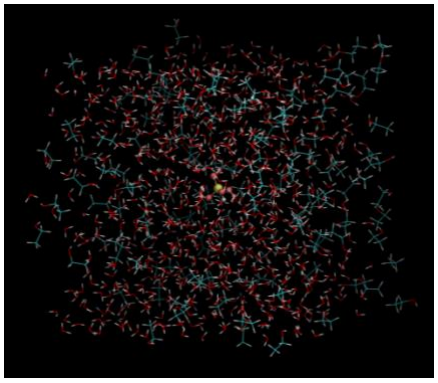

Figure 1: A typical MD snapshot of an orthosilicic acid molecule solvated in water/ethanol heterosolvent.