

## VIENNA COMPUTATIONAL MATERIALS LABORATORY

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## MULTISCALE COMPUTATIONAL TRIBOLOGY

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Tribological processes, e.g. friction and wear, are multiscale phenomena in their nature, i.e. hierarchical in length and time. Therefore tribological systems can be realistically modelled/simulated only in a multiscale fashion, namely by coupling various computational methods, which are highly accurate on their typical length/time scales. Main computational parts of such a multiscale tribological calculation are based on quantum mechanics (QM), molecular dynamics (MD), continuum mechanics (CM) and multibody system dynamics (MBSD), respectively. Although length and time scales overlap to some extent when passing from a computational part to the immediately next one, the main challenge of the multiscale computational tribology still remains the coupling between different levels of modelling.

In the present talk, firstly, some of the well-established approaches and known methods will be extended and used to understand important tribological mechanisms on their relevant time/length scales. Secondly, some of these techniques which are proper on a given scale will be combined into new schemes to cover the hierarchical aspects of various tribological processes.