
화학과 대학원 세미나

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The science and engineering of modern materials from first principles: Anecdotes from in silico experiments

The Materials Theory Group (<https://www.materials-theory.group>) was established in 2010 and our research focuses on the development and application of materials theory for modern-day technologies – in particular, in the fundamental understanding of the chemistry and physics of materials, probed via novel first-principles computational methods (coupled with modern machine-learning methods). By applying state-of-the-art density-functional theory (DFT) calculations and the use of statistical models, simulations of poly-atomic systems are used to understand and predict the structure and properties of solids and their surfaces which includes studying the interactions and reactions of molecules adsorbed on surfaces, and the energetics of defects on surfaces (as well as interfaces) and in the bulk. In this talk, I will provide a brief overview of the past and current research activities conducted in our research group at Yonsei University.

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