

Institutsseminar

Non-traditional Concepts in Chemical Reactivity

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In my talk, I will present two concepts that we have developed in our group. First, I will introduce a concept that goes beyond the traditional relationship between thermodynamics and kinetics, which includes the effect of so-called off-diagonal thermodynamics on reactivity. I will also discuss the applicability of the approach to H-atom transfer chemistry and beyond. Second, I will introduce a concept that goes beyond the traditional Eyring's transition state theory (TST) and employs the analysis of kinetic energy distribution within a reactive mode to understand reaction selectivities that cannot be captured by TST.

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16:15 Uhr

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