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Frontier orbital theory looks at how the transition state of an organic reaction is affected by the interaction of the molecular orbitals of the starting materials. It thus complements the more familiar thermodynamic picture of transition states, in which product-like character is seen as influencing the ease and the course of reactions.

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Frontier orbitals are often considered when trying to understand reactions. The lowest unoccupied molecular orbital (LUMO) may describe an additional electron added to a molecule. An additional electron added to the molecule could have this energy and could be located in the area of space described by this orbital.

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Frontier Orbital Theory A powerful practical model for describing chemical reactivity is the frontier molecular orbital (FMO) theory, developed by Kenichi Fukui in 1950's. The important aspect of the frontier electron theory is the focus on the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO).

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Fukui realized that a good approximation for reactivity could be found by looking at the frontier orbitals (HOMO/LUMO). This was based on three main observations of molecular orbital theory as two molecules interact: The occupied orbitals of different molecules repel each other.

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Frontier orbitals, that is, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), are important indicators for the effect of adsorption on a metal. Due to charge transfer and hybridization, the HOMO-LUMO gap shrinks compared to the free molecule, and the spectroscopic line width of orbital signatures usually increases.

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