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Mechanisms of branching reactions in melanin formation – Ab initio quantum engineering approach – RYO KISHIDA, Department of Applied Physics, Osaka University, SUSAN MEÑEZ ASPERA, HIDEAKI KASAI, National Institute of Technology, Akashi College — Melanin, a pigment found in animals, consists of two types of oligomeric unit: eumelanin and pheomelanin. The color of the skin, the hair, and the eyes is controlled by the ratio of eumelanin/pheomelanin production. Especially, dopachrome and dopaquinone are the precursor molecules of melanin which directly affect the composition of melanin through their branching reactions. Dopachrome is converted into two possible monomers of eumelanin. Dopaquinone can undergo both eumelanin and pheomelanin synthesis. To understand the mechanisms and controlling factors that govern the conversions, reactions of the two molecules are investigated using density functional theory-based first-principles calculations. Our results deepen mechanistic understanding of the reactions and open possibilities to design properties and functions of melanin. In this talk, we will discuss about the competitions of the branching reactions.

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