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Theoretical calculations on the mechanism of local polymerization and depolymerization of C_{60} SHIGERU TSUKAMOTO, MASATO NAKAYA, TOMONOBU NAKAYAMA, MASAKAZU AONO, National Institute for Materials Science, OSAKA UNIVERSITY COLLABORATION, ICORP JST COLLABORATION, UNIVERSITY OF TSUKUBA COLLABORATION — A reversible chemical reaction between C_{60} molecules, polymerization/depolymerization, has been realized and controlled using an STM tip: the polymerization and depolymerization occur at negative and positive sample bias conditions, respectively. Using a first-principles calculation method, we investigated the mechanism responsible for the experimental results. The electronic structures were calculated for polymerized and depolymerized structures of C_{60} dimers under negatively and positively ionized conditions as well as neutral condition. When a couple of C_{60} is negatively ionized, the added electron occupies the initially unoccupied bonding orbital between C_{60} molecules. Then the activation barrier of a polymerization is reduced. When a C_{60} dimer is positively ionized, the bonding orbital energetically approaches to Fermi level and the activation barrier of depolymerization process is reduced.

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