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Title of Doctoral Dissertation

Photoinduced Phase Transitions in Polyacene and Its Heterocyclic Analogs

（ポリアセン及びその複素環式類似体における光誘起相転移）

Photoinduced structure phase transitions in polyacene, paracyanogen and boron-nitride acene are studied. In each compound, there exist two degenerate lattice distorted structure: double bonds in a *cis* pattern and those in a *trans* pattern. In polyacene and paracyanogen, *cis* patterned lattice configurations hold the mirror symmetry while *trans* ones have the C_{2z} rotation invariance. In boron-nitride acene, either *cis* pattern or *trans* pattern has no definite symmetries. We argue that the symmetry properties will strongly affect the optical properties and lead to contrast optical conductivity between the *cis* pattern and *trans*- patterns.

By using the time-dependent Hartree Fock method, we simulate the lattice relaxation process in polyacene, paracyanogen and boron-nitride acene after they are photo excited. We find that photons will induce the lattice fluctuation to preserve the symmetry of the initial state. Due to this symmetry preserving law, phase transitions in polyacene and paracyanogen behaves as a one way switching: Only *trans* patterns can be well converted into *cis* ones, but the reverse conversion is forbidden. Since boron-nitride acene has no definite symmetries in any types of lattice configuration, the symmetry preserving law does not work and the phase transitions between *cis* pattern *trans* pattern is bidirectional.