Broken symmetry states in quasi-one-dimensional molecular conductors
– competitions, co-existences, and frustration –

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Quasi-one-dimensional molecular conductors with a quarter-filled band exhibit a variety of phase transitions, into different electronic and electron-lattice coupled ordered states accompanying symmetry breaking. Typical examples are charge ordering, lattice dimerization (“dimer-Mott” insulator), and spin-Peierls lattice tetramerization [1]. In this talk, a review of our recent theoretical works will be given, which are aiming at elucidating the physical properties of these ordered states and clarifying their competitions and co-existences especially at finite temperatures ($T$), on the basis of one-dimensional (1D) extended Hubbard model.

1) Analytical bosonization + renormalization group studies clarify the critical behavior of the finite-$T$ charge ordering transition, within 1D extended Hubbard chains coupled via inter-chain Coulomb repulsions [2]. By further combining with numerical techniques, $T$ dependence of physical properties such as magnetic susceptibility and electrical resistivity across the transition temperature are computed [3].

2) When the coupling to the lattice degree of freedom is added to the model above, numerical studies show phase competitions/co-existences among the different broken symmetry states [4,5]. The choice of parameters corresponding to different classes of materials brings about different criticalities in its finite-$T$ phase diagrams [5], which can be compared with experimental results.

3) Geometrically frustrated inter-chain Coulomb interaction with a spiral structure, seen in DI-DCNQI\textsubscript{2}Ag, stabilizes a novel “mixed state” of charge order and lattice dimerization, shown by mean-field study on an electron-lattice coupled quasi-1D model [6]. Our results elucidate the mechanism of the ordered state observed in experiments and predict a characteristic $T$ range within the ordered phase, providing a possible reconciliation among puzzling experimental data.