Perspectives for the Ferroelectricity in π-Conjugated Systems.

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Ferroelectricity is a demanded effect in fundamental and applied solid state physics. Till now, the ferroelectrics were known mostly as insulating inorganic materials. In this talk, we discuss a feasibility of obtaining ferroelectric, and the same time electronically and optically active, carbon-based materials: conducting polymers and graphene ribbons. Ferroelectricity related to the charge ordering was discovered in quasi-1D organic conducting crystals $(TMTTF)_2X$ [1], and extended to some layered BEDT based compounds. The interpretation was endorsed by understanding of the "combined Peierls effect" in conducting polymers [2]. In both cases, the microscopic picture is based on two coexisting symmetry lowering effects: dimerizations of bonds and of sites: one of them being build-in, another comes as a spontaneous symmetry breaking. For a searched ferroelectric polymer, with respect to the $(TMTTF)_2X$ case, the origins of these dimerizations will be reversed. One such an $(AB)_x$ polymer has been already announced and studied for nonlinear optical properties [3], but not tested yet for the low frequency response which could have recovered the ferroelectricity. The theory [2] predicts an existence of solitons with non-integer variable charges, both with and without spin, which are the walls separating domains with opposite electric polarisation. Their physics will serve to relate transient ferroelectric processes and the visible-range optics. For ribbons of graphenes, the zigzag edges possess the build-in dimerization of sites edge carbon atoms, while the spontaneous one may come from electron-phonon interactions.

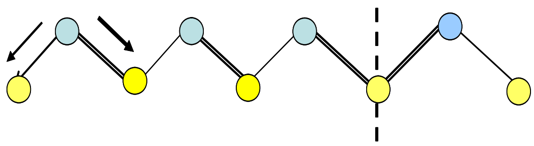

Fig. Joint effect of extrinsic Δ_{ex} and intrinsic Δ_{in} contributions to dimerization gap Δ. Δ_{ex} comes from the build-in site dimerization – non equivalence of sites A and B. Δ_{in} comes from spontaneous dimerization of bonds - the Peierls effect.

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[3] L. Luer et al, Chem. Phys. Lett. **444**, 61 (2007) and refs. therein.