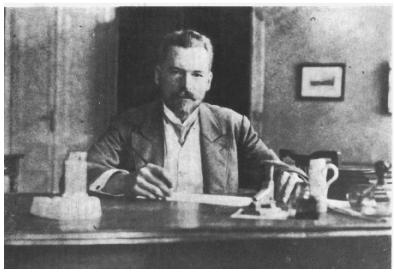

Contribution ID: **38** Type: **Poster**

Splay modulation in a system composed of hard wedges

We studied equilibrium systems composed of wedge-shaped monodisperse molecules using hard-particle Monte Carlo simulations. Each model molecule was made up of six colinear tangent spheres with linearly decreasing diameters. Thus, the shape was unequivocally described by a single parameter d: the ratio of the smallest and largest diameters of the spheres. The phases of the systems were analyzed as a function of d and packing density η. As interactions were purely of the excluded volume type, the emergent phases were governed solely by the configurational entropy. For $\eta < 0.5$, in addition to the isotropic liquid, we observed standard nematic and smectic A liquid crystalline phases. However, for $\eta > 0.5$, apart from the ordinary non-polar hexagonal crystal, three new frustrated polar crystalline phases with splay modulation appeared: ferroelectric double splay crystal ($\mathrm{Cr_{DS}P_F}$), antiferroelectric double-splay crystal ($\mathrm{Cr_{DS}P_A}$), and antiferroelectric splay crystal ($\mathrm{Cr_SP_A}$). All configurations were studied in terms of nematic, smectic, and hexatic order parameters, as well as the radial distribution function and the polarization correlation function. In addition, we conducted bifurcation DFT analysis in search of polar liquid crystalline structures. It confirmed the numerical results where long-range polar correlations are present only in the solid phase.

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Session Classification: Poster Session and Coffee