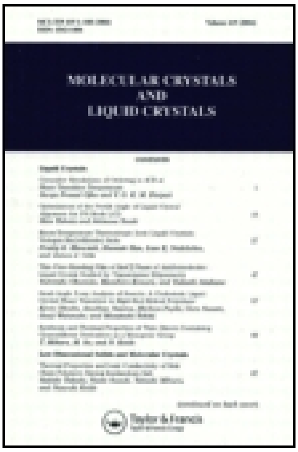

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Theoretical Predictions and Comparison with Neutron Scattering Experiments for Liquid-Crystalline Polymers

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Theoretical Predictions and Comparison with Neutron Scattering Experiments for Liquid-Crystalline Polymers

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A summary of new theoretical predictions and results from *unique* microscopic, molecular statistical-physics theories[1–3] for backbones and side chains of liquid-crystalline polymers (LCPs) is presented for pure (single-component) systems and for mixtures.

The results calculated from these theories are in *very* good agreement (from zero deviations to less than about 6% relative deviations) with available experimental data, including recent data from neutron scattering experiments[4] for side-chain LCPs. This data includes (1) transition temperatures involving nematic (*N*) and smectic (*S*) LC phases and the isotropic (*I*) liquid phase and (2) quadratic characteristic radii $R_{\parallel}$ and $R_{\perp}$ of the LCPs parallel and perpendicular, respectively, to the nematic director when the side chains of these LCP molecules are aligned parallel to each other in an applied magnetic field.

The results from these theories extend significantly beyond the information available from present experiments (including present neutron scattering experiments). That is, these theories also give (1) predictions of details of the microscopic orderings and arrangements of the backbones and side chains of these side-chain LCP molecules on different length scales in the various phases and (2) physically satisfying explanations for these arrangements. Some of these theoretical predictions are now being tested in new neutron scattering experiments in France.

These theories have *no* ad hoc or arbitrarily adjustable parameters. The input variables in these theories are taken from experimental data for atoms or small chemical groups such as benzene rings and methylene groups.

Thus, these theories have been used to theoretically design (atom by atom, bond by bond) entirely new LCP (and solvent) molecules to then chemically synthesize. This theoretical research[1–3] includes the prediction and molecular design of the first super-strong LCPs (first LCPs with good compressive strengths as well as with tensile strengths and tensile moduli significantly better than existing LCPs, such as Kevlar) and their solvents. The chemical syntheses of some of these theoretically designed super-strong LCPs are in progress at multiple research institutions.

Relative phase stabilities (involving *N* and multiple *S* LC phases and the *I* liquid phase), thermodynamic and molecular ordering properties (including odd-even effects and radii of gyration), and some dynamic and mechanical properties have been calculated with these theories for various kinds of LCPs as a function of pressure, temperature, degree of polymerization, and side-chain and repeat-unit chemical structures (including bond lengths and angles, intra-chain rotation energies, pair potentials, dipole moments, polarizabilities, etc.). These theories have predicted and explained different kinds of ordering, including local smectic-A (SA) ordering in the side chains of LCPs.

There is a very real need to perform many more neutron scattering experiments on LCPs (both side-chain LCPs, as well as other kinds of LCPs) and to compare the additional experimental results with the predictions of these theories here.

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