Supporting Information for

Remarkable order of a high-performance polymer

*Christopher J. Takacs[#], Neil D. Treat[†], Stephan Krämer[+], Zhihua Chen[§], Antonio Facchetti[§], Michael L. Chabinyc[‖], Alan J. Heeger[#,]**

[#] Department of Physics, Broida Hall, University of California, Santa Barbara, Santa Barbara, California 93106, United States

[§] Polyera Corporation, Skokie, IL 60077

[+] Materials Department, University of California Santa Barbara, Santa Barbara, California 93106, United States

[†,‖] Materials Research Laboratory, Materials Department, Mitsubishi Chemical Center for Advanced Materials, University of California Santa Barbara, Santa Barbara, California 93106, United States

Corresponding Author

* ajhe@physics.ucsb.edu

Present Addresses

† Department of Materials, Imperial College London, London SW7 2AZ

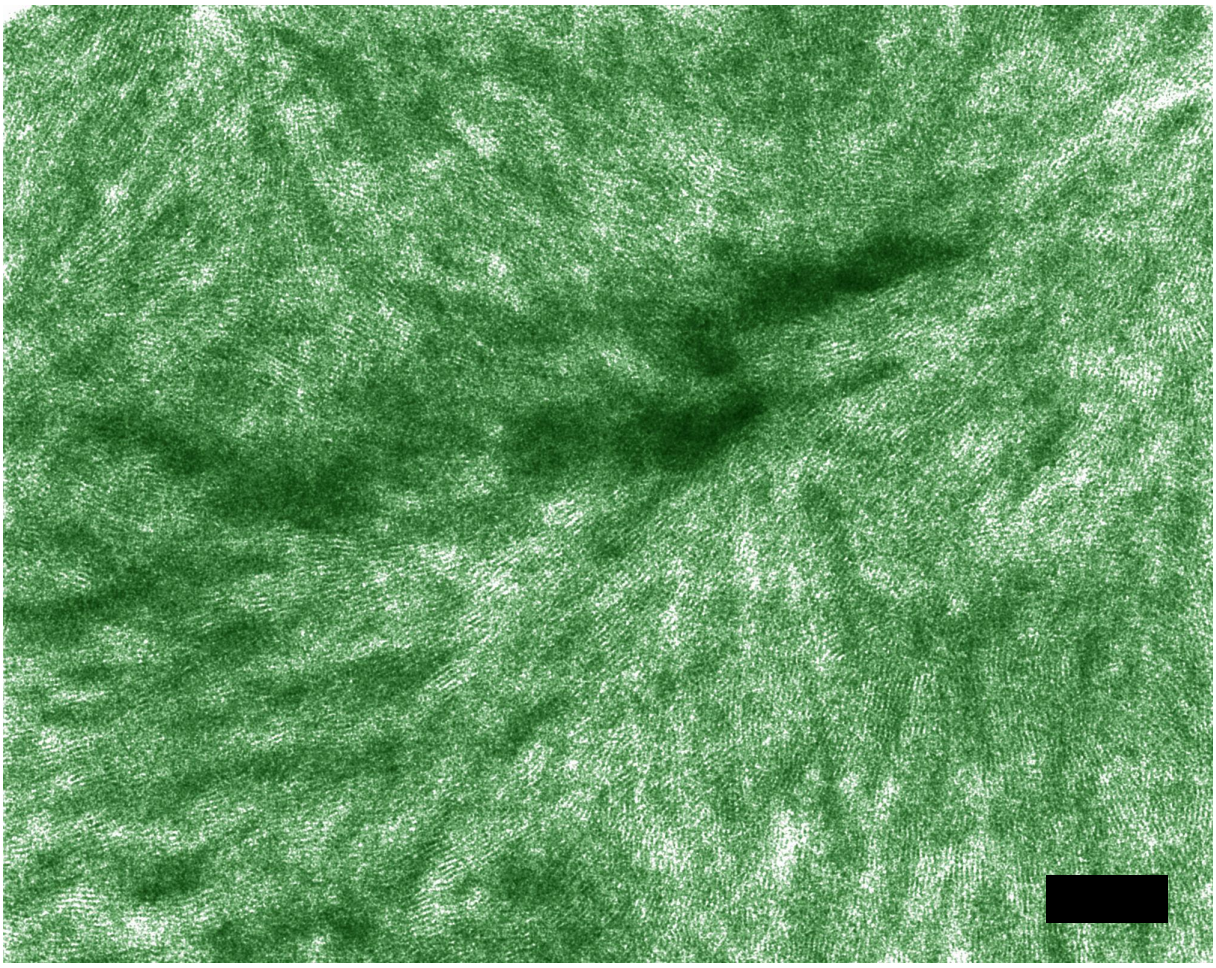

Figure S1. STEM image. Scale bar is 50 nm.

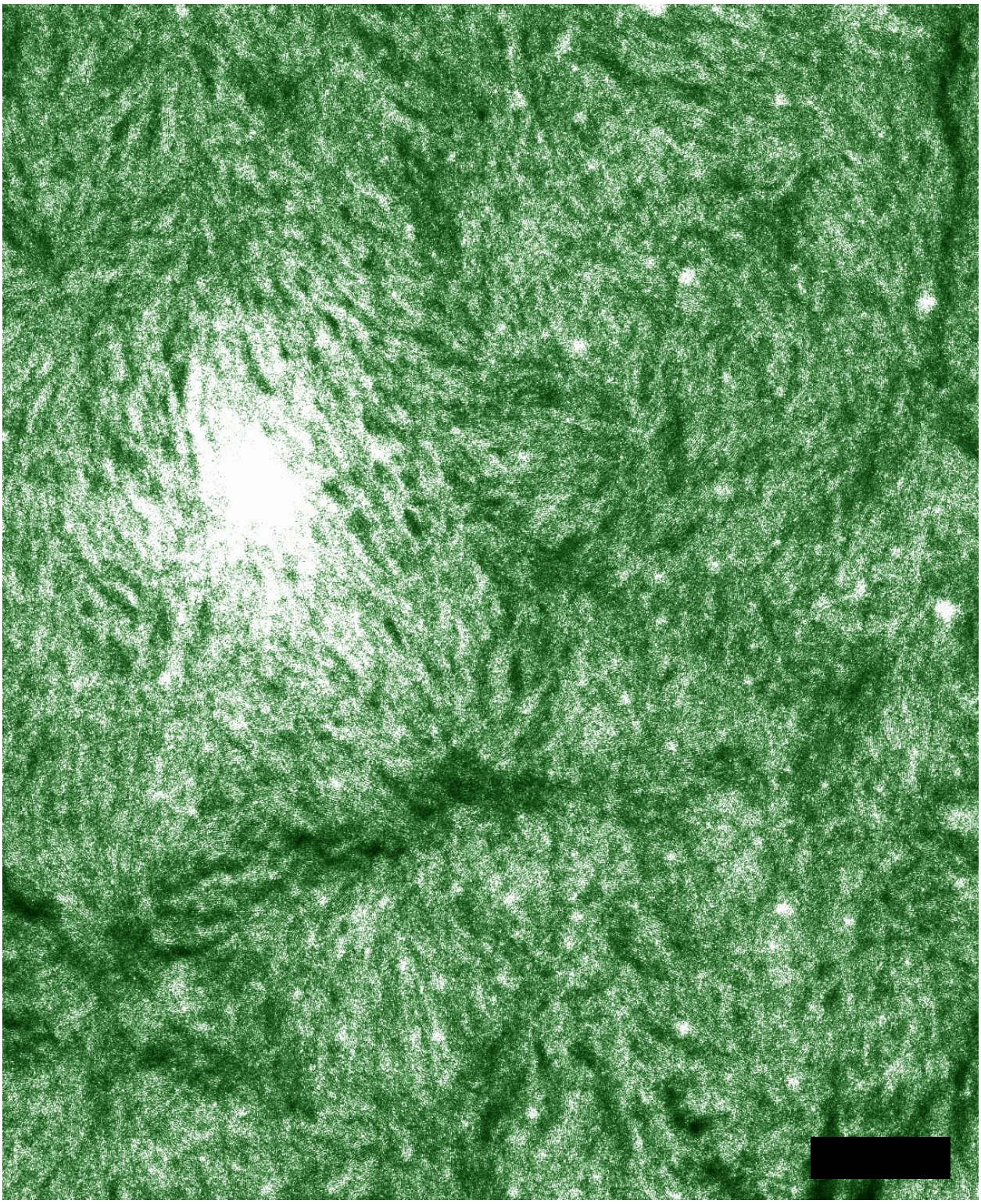

Figure S2. STEM image of a larger area. Scale bar is 200 nm.

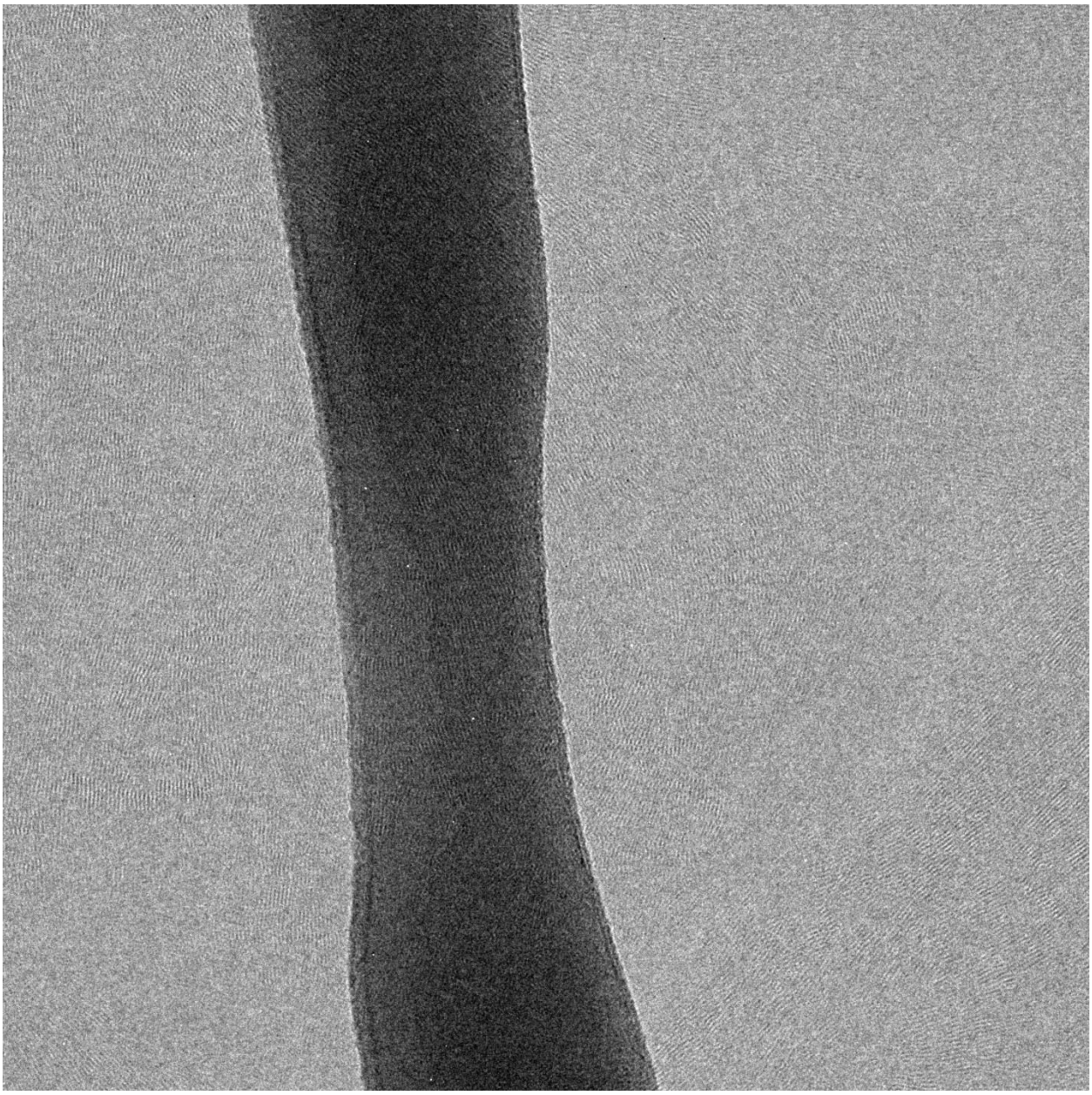

Figure S3. Raw HRTEM image showing alkyl lattice planes. The dark strip is part of the TEM grid and not a feature of the sample. The image is 650 nm by 650 nm.

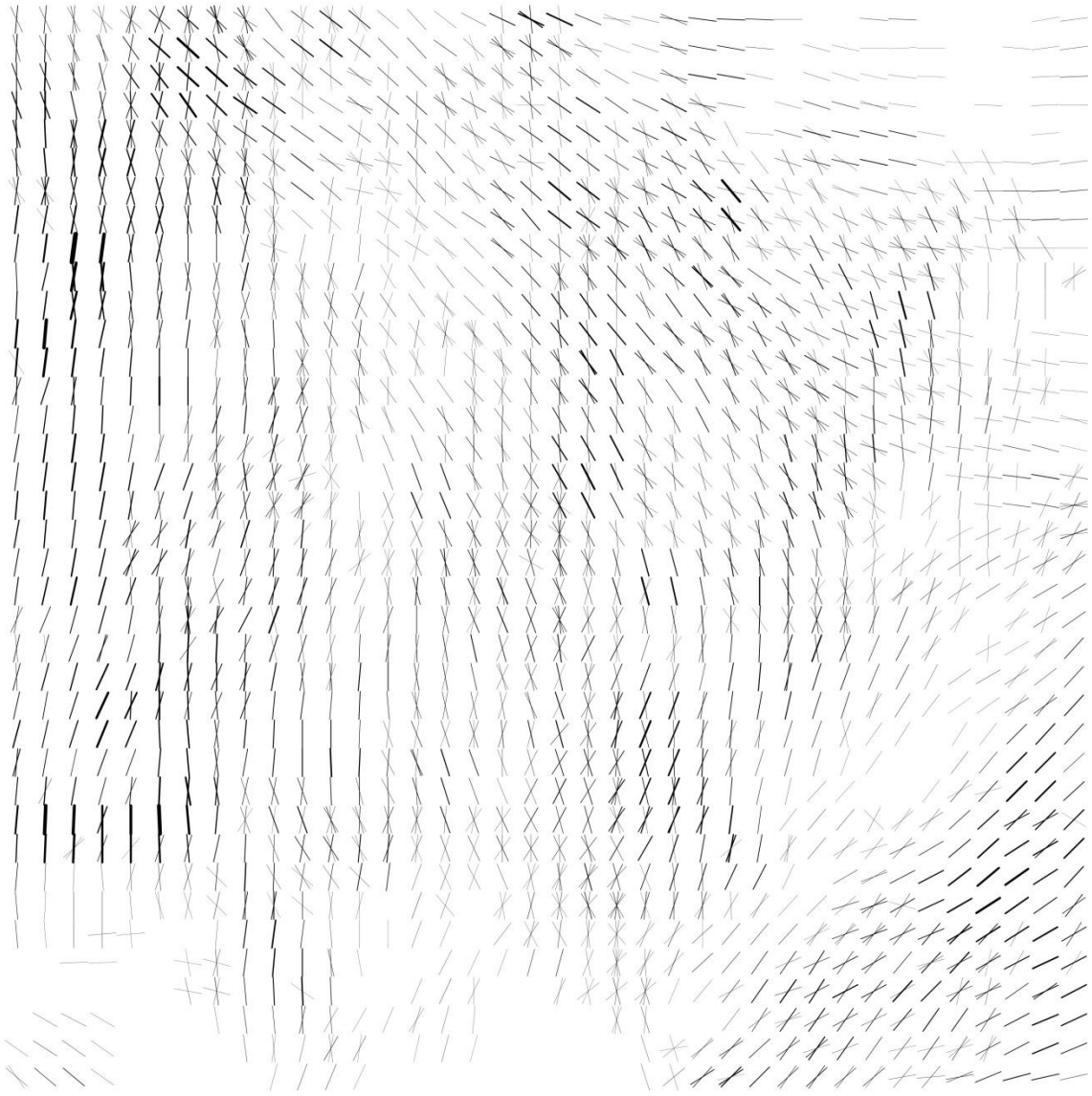

Figure S4. Director field computed from the HRTEM image. The width of the lines is proportional to the strength of the observed order.

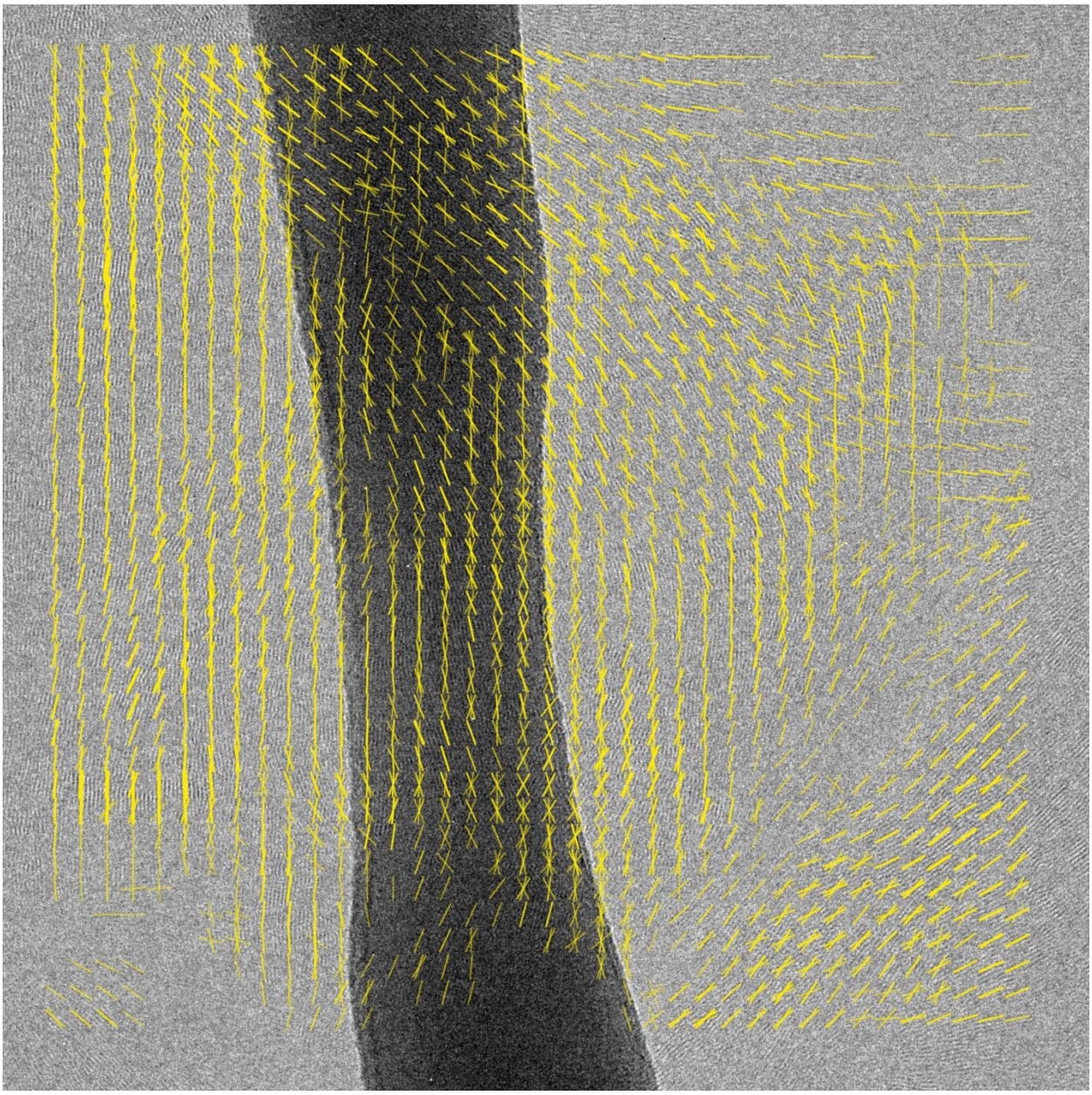

Figure S5. Director field overlaid on the HRTEM image.

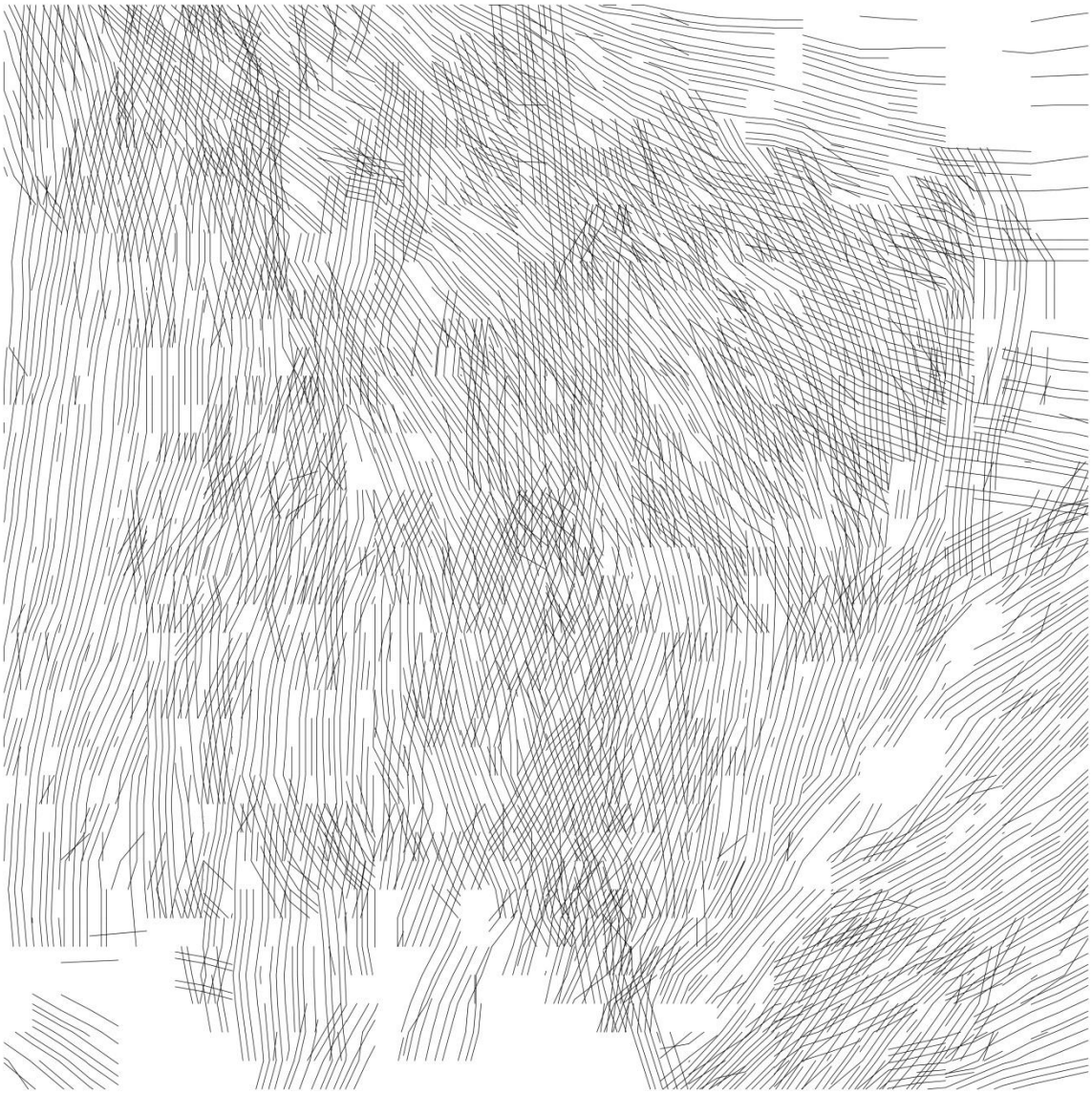

Figure S6. Integrated director field.

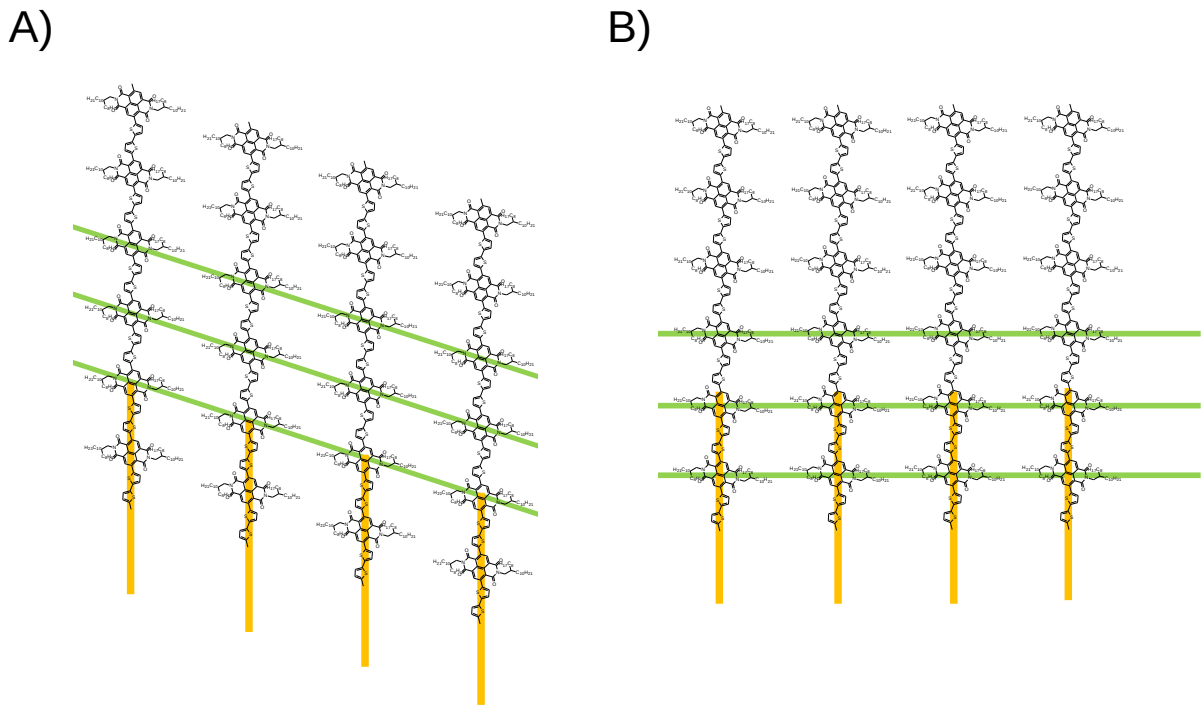

Figure S7. An illustration of how local slippage of the backbones from A) to B) can change the direction of the (001) and higher order reflections relative to the (100). The (100) lattice planes are shown in orange with the (001) is shown in green. We note the structure factors of the reflections will also change with slippage and orientation of the monomers in the backbone.

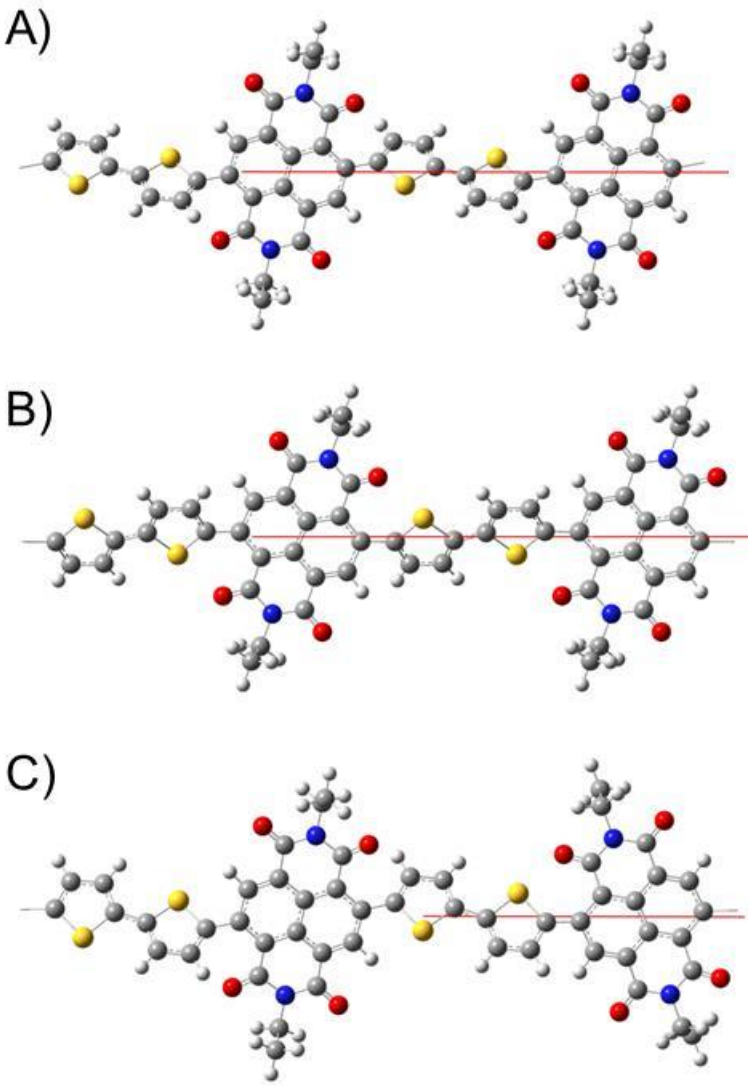

Figure S8. Three possible linear conformations of P(NDI2OD-T2) with the side-chains omitted. The thiophenes in all configurations are tilted out of the plane with respect to the NDI units. Configuration A) is predicted to be the ground state with B) and C) predicted to be 54 meV and 27 meV higher in energy, respectively. Calculations and geometry optimization were performed in the gas-phase at a RB3LYP/6-311G(d,p) level of theory using Gaussian09.[1] The red lines represent the center of the polymer backbone.

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.;

Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision B.01. Wallingford CT, 2009.