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First-principles study of polythiophene and polyselenophene crystals for organic electronics[1] TAKAO TSUMURAYA, JUNG-HWAN SONG, A.J. FREEMAN, Northwestern University — Semiconducting polymers, like regioregular poly(3-hexylthiophene)/poly(3-hexylselenophene) (rr-P3HT/rr-P3HS) are currently the most widely studied materials in a variety of applications for polymer based bulk-heterojunction (BHJ) solar cells and organic field-effect transistors (OFET). [1,2] For both applications, the performance of devices has been attributed to thin film structures of rr-P3HT/rr-P3HS on substrates. To understand their mechanisms, the crystal structure has been extensively investigated by using various experimental techniques. However the crystal structure has yet to be unambiguously characterized. Here, we proposed several possible structures and investigated their stabilities from first-principles density functional calculations based on the all-electron FLAPW method. [3] We found that two base-centered monoclinic structures belonging to space group $A2$ are in the degenerate lowest energy structures. The electronic and transport properties are also discussed. Lastly, we report on the differences in electronic and crystal structure between rr-P3HT and rr-P3HS.

[1] G. Li *et al.*, Nature Mater. **4**, 864 (2005).
[2] H. Sirringhaus *et al.*, Nature **401**, 685 (1999).
[3] E. Wimmer *et al.*, Phys. Rev. B **24**, 864 (1981).

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