PBC-DFT : An Efficient Method to Calculate Energy Band Gaps of Conducting Polymers used in Solar Cells

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Background

Conventional crystalline silicon solar cells are approximately 20% efficient. However, silicon solar cells are costly to make relative to other forms of renewable energy. Solar cells produced with organic conducting polymers offer a great alternative to silicon solar cells because of their ease of processing and potential for low cost production. In order to become marketable organic solar cells need to achieve efficiencies of 10% or higher.

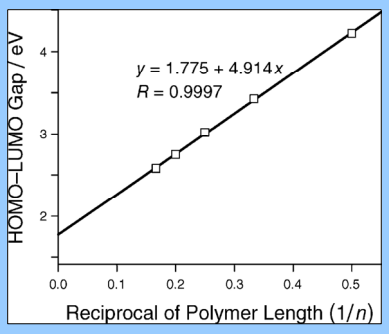
•The general structure of a conducting polymers used in most organic solar cells today consists of a donor and an acceptor group in a copolymer.

• After an initial photoexcitation, electrons are transferred from the copolymer donor to an acceptor (typically a fullerene material). The separated charges can then migrate to the respective electrodes to generate power.

• This research focused on the properties of the copolymer donor. The energy difference between the HOMO and the LUMO of these materials is referred to as the energy band gap.

• Smaller band gaps (<1.8 eV) in conducting polymers typically lead to higher performing efficiencies.

•In the past band gaps have been found using theory by calculating the energy gaps of increasing oligomer lengths (n), then plotting the reciprocal oligomer length (1/n) as a function of the HOMO-LUMO gap (in eV) .



• This data was extrapolated to the y-intercept which gives the band gap of the polymer:

PBC-DFT

• Periodic boundary conditions (PBC) treats the polymer as a one-dimensional unit cell

• Calculations converge to find the lowest energy state and HOMO/LUMO values

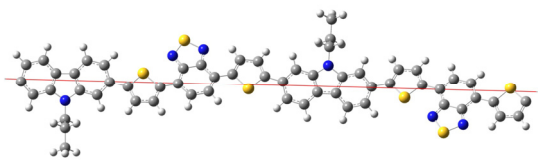
• The advantage of PBC is one calculation is run versus the multiple calculations needed for the 1/n method

Method

• Gaussian 03 software was used with GaussView as the graphical interface

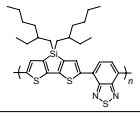
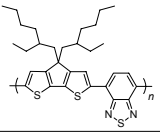
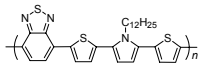
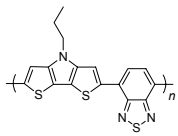
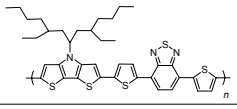
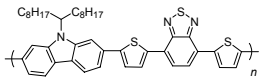
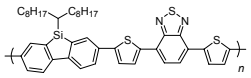
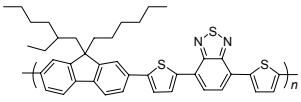
• Method: density functional theory using B3LYP/3-21G(*)

• An optimized dimer was used to define the unit cell for all PBC-DFT calculations



Example of a dimer unit cell PBC calculation in Gaussian 03 for **P7**

Results

Structure	Polymer (ref)	PCE (%)	E_g (eV) Optical	E_g (eV) Echem	PBC-DFT (eV) HOCO (LUCO)	E_g (eV) PBC-DFT
	P14	5.10	1.45	1.78	-4.44 (-2.99)	1.44
	P13	5.50	1.40	1.73	-5.63 (-4.33)	1.33
	P1	1.00	1.60	1.77	-4.76 (-2.78)	2.12
	PDTP-BTcis	N/A	1.4	1.87	-4.33 (-2.97)	1.36
	P9	2.18	1.46	1.57	-4.52 (2.80)	1.73
	P7	3.60	1.88	1.90	-4.87 (-2.75)	2.12
	P8	1.60	1.85	1.89	-4.93(-2.80)	2.13
	P4	2.20	N/A	N/A	-4.93(-2.80)	2.26

Conclusions

• Calculation time was saved relative to the 1/n method

• PBC-DFT provided band gaps in excellent agreement with experimental data for fused donors; non-fused donors provided greater deviations from experimental data

• Calculations for these polymers can be performed to screen potential materials

References

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