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Novel Absorber Material Design Based on Thiazole Derivatives Using DFT/TD-DFT Calculation Methods for High-Performance Dye Sensitized Solar Cell

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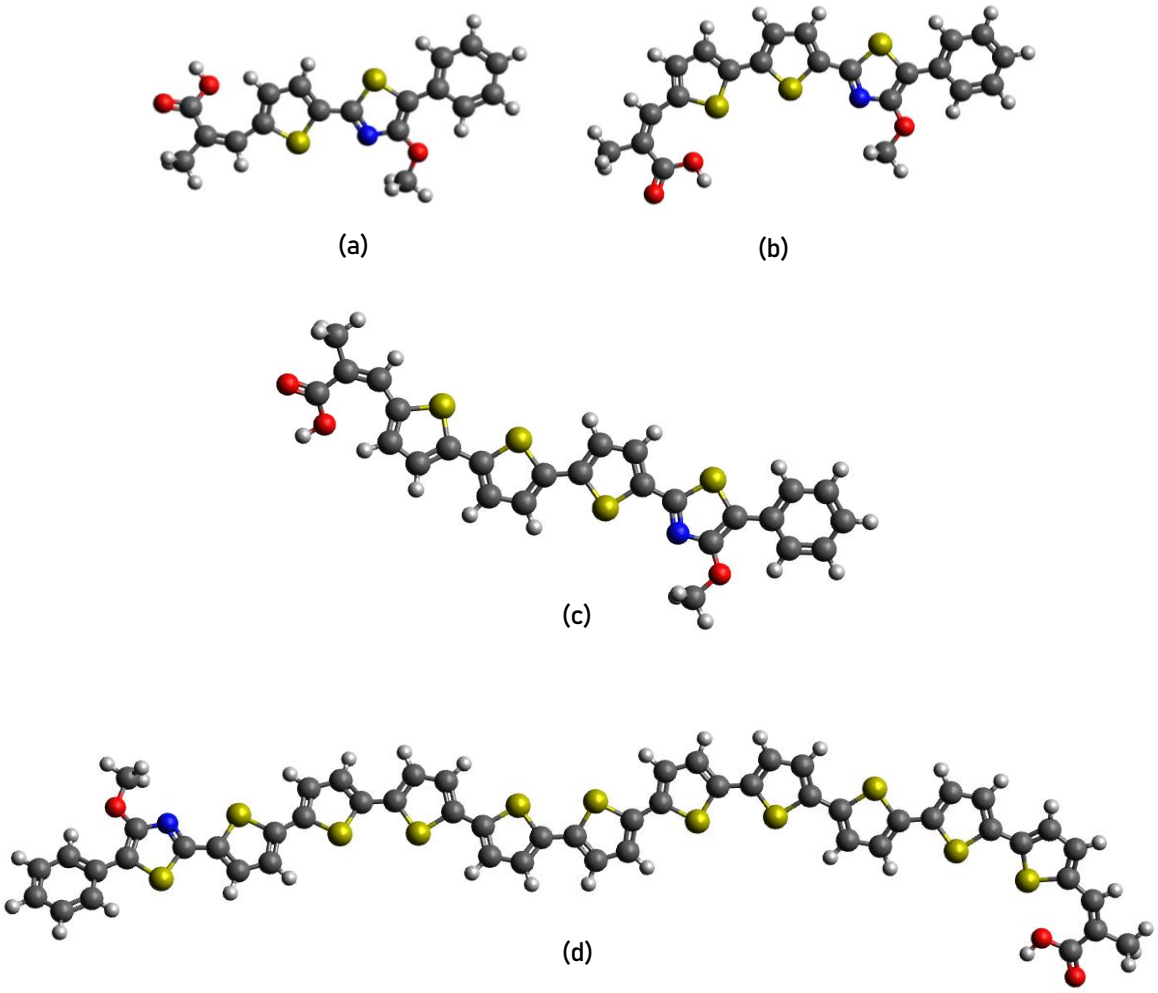

Fig. S1. Optimized structure of thiazole derivatives with variation of 1 (a), 2 (b), 3 (c), and 10 (d) number of thiophenes.

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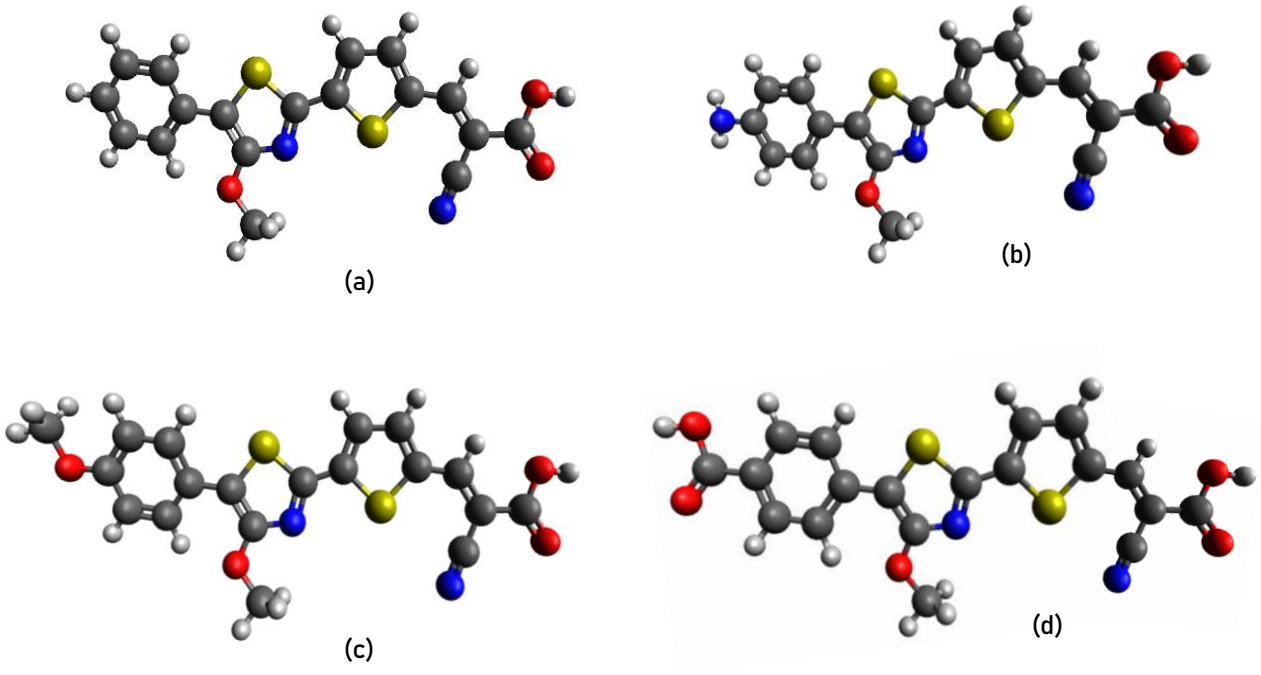

Fig. S2. Optimized structure of thiazole derivatives with variation of –H (a), -NH_2 (b), -OCH_3 (c), dan –COOH (d) molecules.

Table S1. Energy of the optimized structure of thiazole derivatives with variation of –H, -NH_2, -OCH_3, and –COOH molecules.

Variation molecule	Total SCF Energy (Hartree)	Total SCF Energy (kJ mol^{-1})
-H	-1824.63	$-4.79x10^{-8}$
-NH_2	-1879.98	$-4.93x10^{-8}$
-OCH_3	-1939.16	$-5.09x10^{-8}$
-COOH	-2013.23	$-5.28x10^{-8}$