

Supporting Information: Ionic association in
 $\text{CH}_3-(\text{CH}_2-\text{CF}_2)_n-\text{CH}_3(\text{PVDF})-\text{Li}^+-(\text{CF}_3\text{SO}_2)_2\text{N}^-$
for n=1,4: A computational approach

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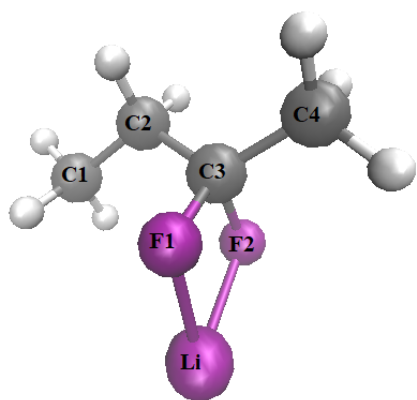
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Table S1: Zero-point corrected electronic (E in AU) and relative stabilization energy (ΔE in kJ/mole) of conformers of $\text{CH}_3-(\text{CH}_2-\text{CF}_2)_n-\text{CH}_3$ (n=1-4)

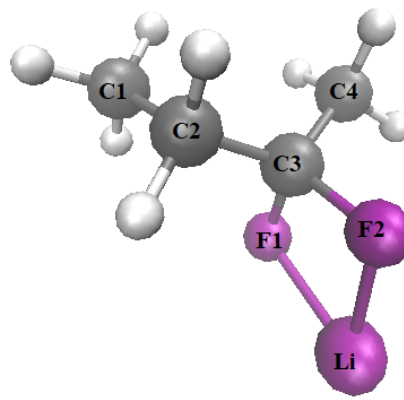
System	E	ΔE
M1	-356.8354	0
M2	-356.834589	2.13
D1	-633.904027	0
D2	-633.898765	13.82
T1	-910.971566	0
T2	-910.961657	26.02
Te1	-1188.03966	0
Te2	-1188.036581	8.08
Te3	-1188.033567	16
Te4	-1188.024471	39.88

Table S2: Electronic (E in AU) and relative stabilization energy (ΔE in kJ/mole) of conformers of $\text{CH}_3-(\text{CH}_2-\text{CF}_2)_n-\text{CH}_3$ (n=1) obtained from different methods

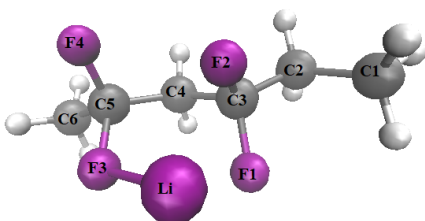
Method	M1 (g) (in au)	M2 (t) (in au)	M1-M2 (in kJ/mole)
B3LYP/6-31G**	-356.952197	-356.951410	-2.07
B97D/6-31G**	-356.762149	-356.761903	-0.65
B3LYP/6-31++G**	-356.975534	-356.975904	0.97
MP2/6-31G**	-355.034623	-355.035656	2.71



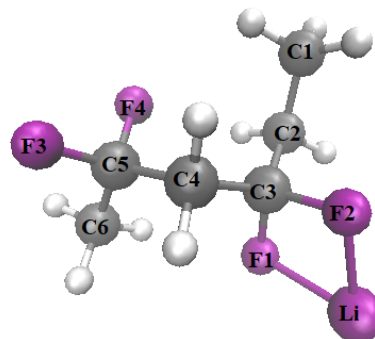
C11



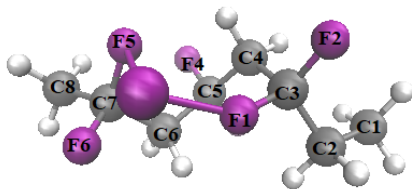
C12



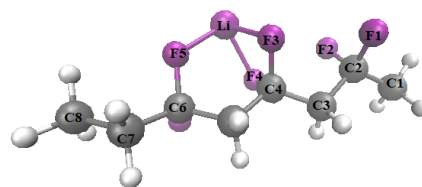
C21



C22

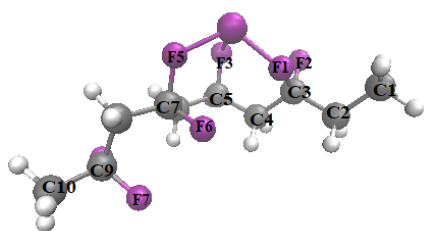


C31

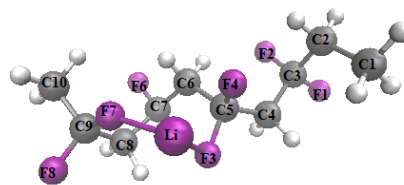


C33

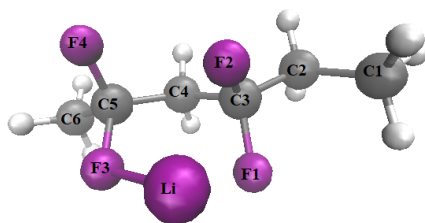
Figure S1: Optimized geometries of different conformers of $\text{Li}^+ \text{-CH}_3 \text{-(CH}_2 \text{-CF}_2)_n \text{-CH}_3$ ($n=1-3$).



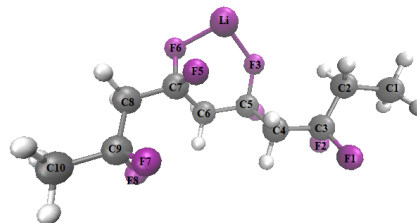
C41



C42



C43



C44

Figure S2: Optimized geometries of different conformers of $\text{Li}^+\text{-CH}_3\text{-(CH}_2\text{-CF}_2\text{)}_4\text{-CH}_3$.