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Similar results between LAMMPS codes and Nielson et al.

Identical results between both LAMMPS codes

TABLE 1: Relative Energies for All-Carbon Phases

	LAMMPS (Feb 11 2011)		Nielson et al.	
Compound	Ereax (kcal/mol)	Ereax/c (kcal/mol)	Eref (kcal/mol)	EReaxFF (kcal/mol)
Graphite	0.00	0.00	0.00	0.00
Graphene	1.57	1.57	1.30	1.56
10_10 Nanotube	2.72	2.72	2.80	2.83
C60 Buckyball	11.44	11.44	11.50	11.30

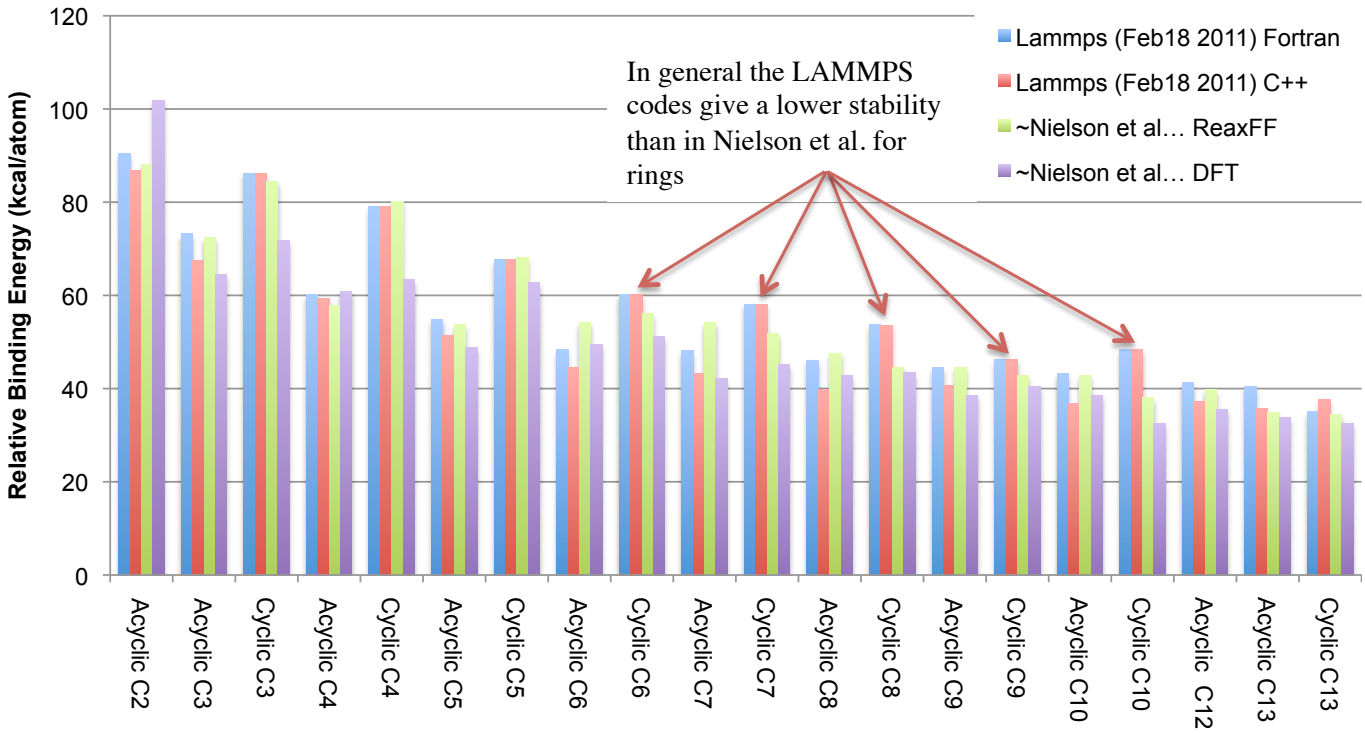
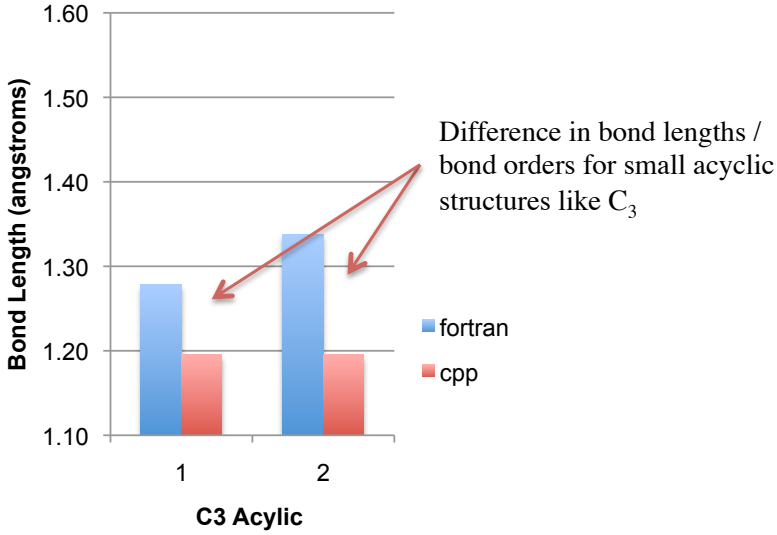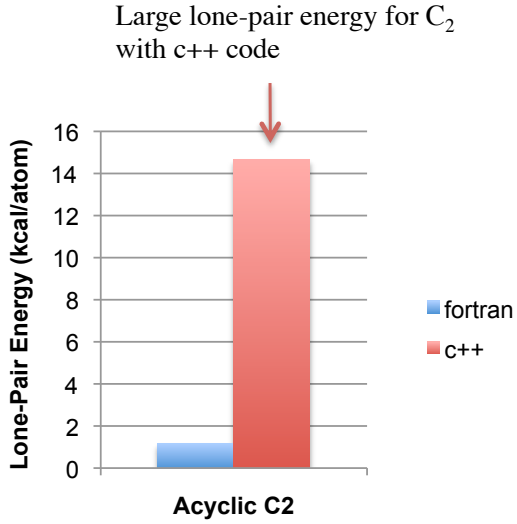
Figure 1. DFT and ReaxFF relative stabilities for small all-carbon fragments.