UNDERSTANIDNG MOLECULAR TRANSPORT IN CARBON NANOTUBES

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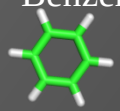
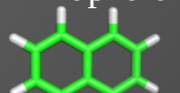
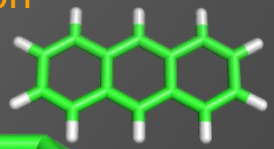
- With only two atomic polarizability parameters, we are able to reproduce the **molecular polarizability tensors** of a series aromatic compounds including carbon nanotubes







		α_x	α_y	α_z
Benzene	Expt	11.70	11.70	5.72
	Expt	12.26	12.26	6.66
	Model	12.00	12.00	6.67
Naphthalene	Expt	20.20	18.80	10.70
	Expt	22.20	18.20	7.30
	Model	22.08	18.41	9.94
Anthracene	Expt	35.20	25.60	15.20
	Expt	44.70	25.80	9.80
	DFT(B3LYP/6-31G*)	38.65	21.65	6.51
	Model	33.78	24.42	13.25
Nanotube (3,3)	DFT(B3LYP/6-31G*)	59.65	39.06	39.06
	DFT(B3LYP/6-31+G*)	64.45	47.33	47.33
	Model	63.82	42.88	42.88

- REMD simulations show that poly gly-lac may exist in both left-handed (a) or right-handed (b) helical conformations in solution. While poly lys-lac (c) is more likely to adopt an extended polyproline II structure.