S. Konduri, S. Mukherjee, and S. Nair, **"**Controlling Nanotube Dimensions: A Correlation between Composition, Diameter, and Internal Energy of Single-Walled Mixed Oxide Nanotubes"

A) Gaussian fit to FTIR spectra of AlSiGeOH nanotubes

In order to quantify the Ge to Si ratio in the mixed metal oxide nanotubes a rigorous curve fitting procedure was developed. Firstly, the pure nanotube (Al-Ge and Al-Si nanotube) spectra were fitted to minimum number of Gaussians to obtain an accurate fit. Then, keeping the peak positions fixed and varying the intensity and peak widths of all the Gaussians in the pure nanotube spectra, all the respective AlSiGeO nanotube spectra was fitted. The peak fits for the mixed metal oxide nanotubes are shown in Supporting Figure 1. The Ge and Si peak areas in the AlSiGeOH nanotubes are shown in Supporting Table 1, along with the Ge content of the nanotubes calculated from the areas of the fitted peaks.

Molar composition of Ge in precursor solution (1-x)	FTIR Analysis Results		Molar composition of Ge in Nanotube product
	Total area from:		
	Si-O vibrations	Ge-O vibrations	
1.0	72.44	0.00	1.0
0.75	149.52	54.38	0.7333
0.6875	118.52	46.10	0.72
0.625	121.39	93.83	0.564
0.5	153.62	148.91	0.5078
0.25	60.73	219.03	0.217
0.0	0.00	124.94	0.0

Supporting Table I. Fitting results of FTIR spectra of mixed metal oxide nanotubes and composition calculations.
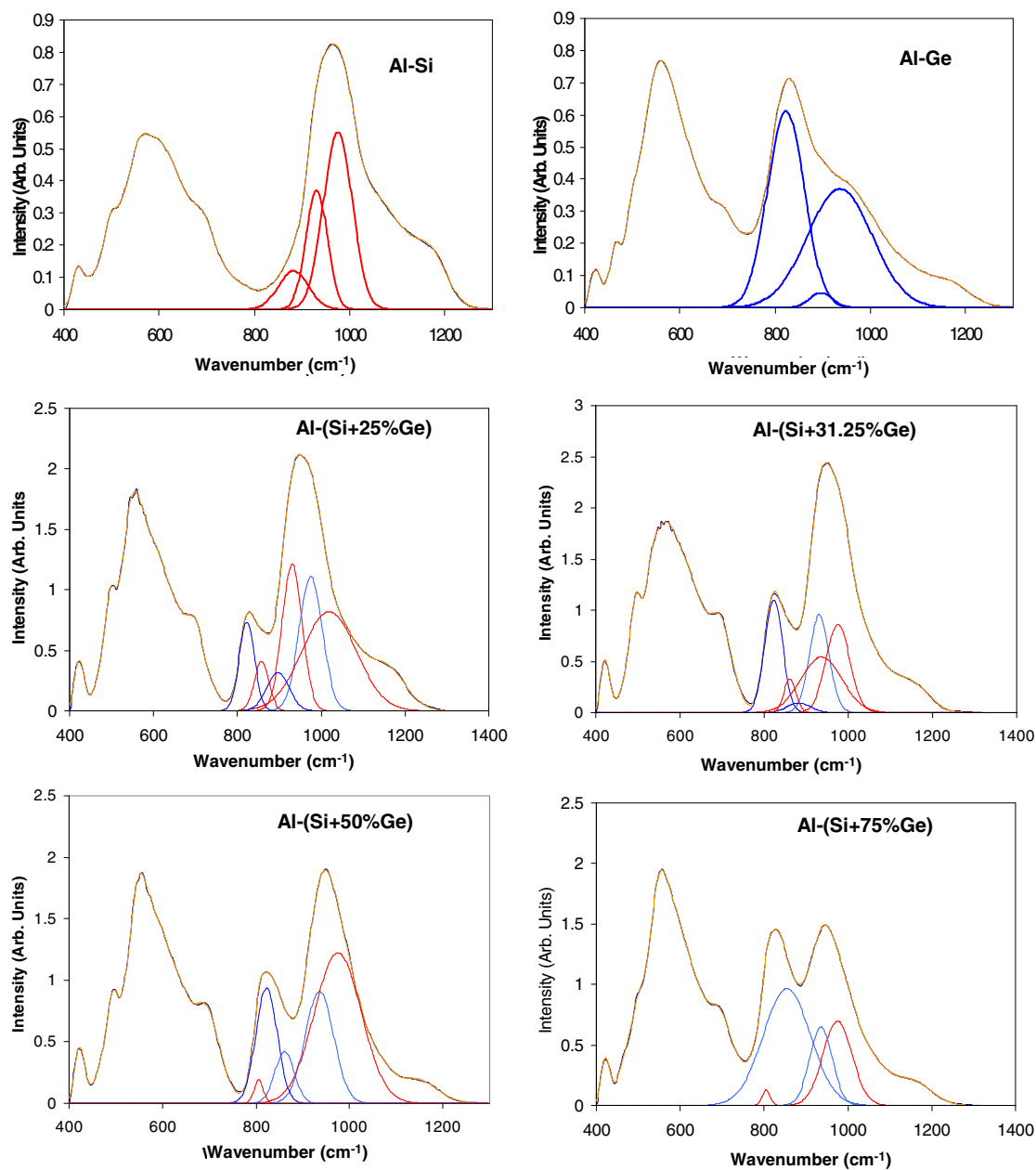
Supporting Figure 1: Fitted FTIR spectra of mixed metal oxide nanotubes. The Gaussian curves indicated in red are Si-O vibrations and blue are Ge-O vibrations.

B) Comparison of simulated structural properties of C-phase of Na{AlGeO₄}, D-phase of K{AlGeO₄} and α- GeO₂ with experimental crystal structure data

Supporting Table II shows the results of geometry optimizations on C-phase of Na{AlGeO₄}, D-phase of K{AlGeO₄} and α- GeO₂ using the final fitted force field parameters (Table I in the main paper). The energy minimization simulations were performed with steepest descent followed by conjugate gradient algorithms until the maximum energy gradient at any atom was below 1 kcal/mol/Å. The values of Al-O and Ge-O bond lengths were obtained by averaging over all the Al-O and Ge-O bonds present in the crystal structure. The results suggest very good agreement between the force field predictions and the experimental crystal structure data. The only properties with significant deviation between prediction and experiment were the b-axis and c-axis values for the C-phase and D-phase respectively, which deviate by 1.8% and 3% respectively. However, the force field could not be refined further within the framework of the CLAYFF potential energy expression.

	C-phase of Na{AlGeO₄}		D-phase of K{AlGeO₄}		α- GeO₂	
	Simulation	Experimental	Simulation	Experimental	Simulation	Experimental
a (Å)	8.671	8.783	18.416	18.429	4.923	4.985
b (Å)	15.139	15.432	18.416	18.429	4.923	4.985
c (Å)	8.272	8.252	8.882	8.599	5.617	5.648
α (deg)	90	90	90	90	90	90
β (deg)	90	90	90	90	90	90
γ (deg)	90	90.1	120	120	120	120
ρ (g/cc)	3.42	3.32	3.10	3.19	4.42	4.29
Al-O	1.738	1.751	1.747	1.747	----	----
Ge-O	1.732	1.741	1.727	1.745	1.744	1.738

Supporting Table II: Comparison of simulated (using final FF parameters) structural properties of C-phase of Na{AlGeO₄}, D-phase of K{AlGeO₄} and α- GeO₂ with experimental crystal structure data.

C) Comparison of experimental IR and calculated power spectra of AlSiGeOH Nanotubes

In order to provide a direct comparison between the experimental IR and calculated vibrational spectral position assignments, the computed power spectra of the nanotubes were fitted with a minimum number of Gaussians functions to determine the exact positions of the vibrational peaks. The fitting procedure detailed above in Section A was adopted to obtain the peak positions for the pure nantubes i.e. AlSiO, AlGeO and for mixed nanotube AlSiGeO with x = 0.5. The peak fits for the mixed metal oxide nanotubes are shown in Supporting Figure 2.
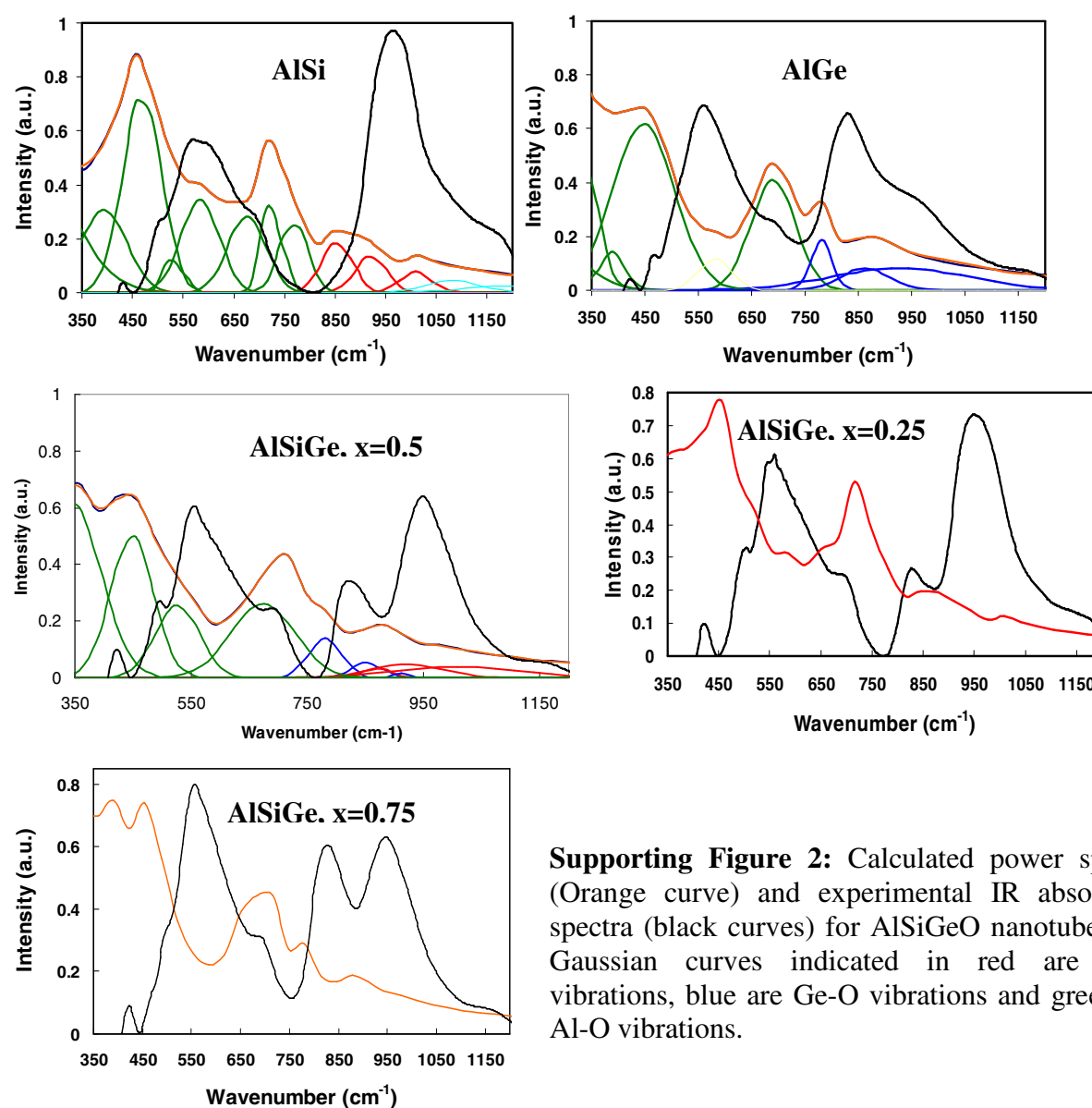
Supporting Figure 2: Calculated power spectra (Orange curve) and experimental IR absorption spectra (black curves) for AlSiGeO nanotube. The Gaussian curves indicated in red are Si-O vibrations, blue are Ge-O vibrations and green are Al-O vibrations.