

## Supplementary Information

### Broadband terahertz signatures and vibrations of Phe-Phe peptide and its fibrils

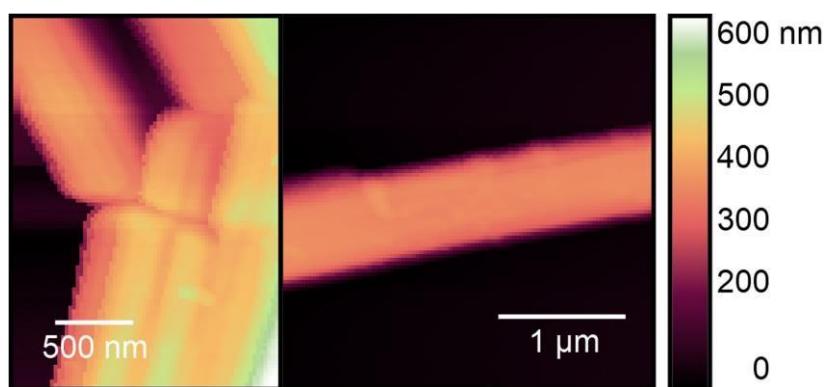
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**Fig. 1S** AFM topography map acquired on f-Phe-Phe fibrils, revealing rod-like aggregated structures having thicknesses of approximately 300 nm.

#### DFT Simulations

<b>Functional</b>	<b>Basis</b>		
<b>B3LYP</b>	<b>6311Gd</b>	<b>6311Gdp</b>	<b>6311Gdp++</b>
	0.14	0.27	0.26
	0.24	0.34	0.37
	0.47	0.54	0.56
	0.70	0.66	0.65
	0.78	0.78	0.93
	0.98	1.00	1.06
	1.84	1.84	1.77
	2.11	2.2	2.01
	2.46	2.45	2.45
	3.86	2.79	2.82

**Table. 1S Simulated normal modes analysis of Phe-Phe obtained with different set of bases.**