

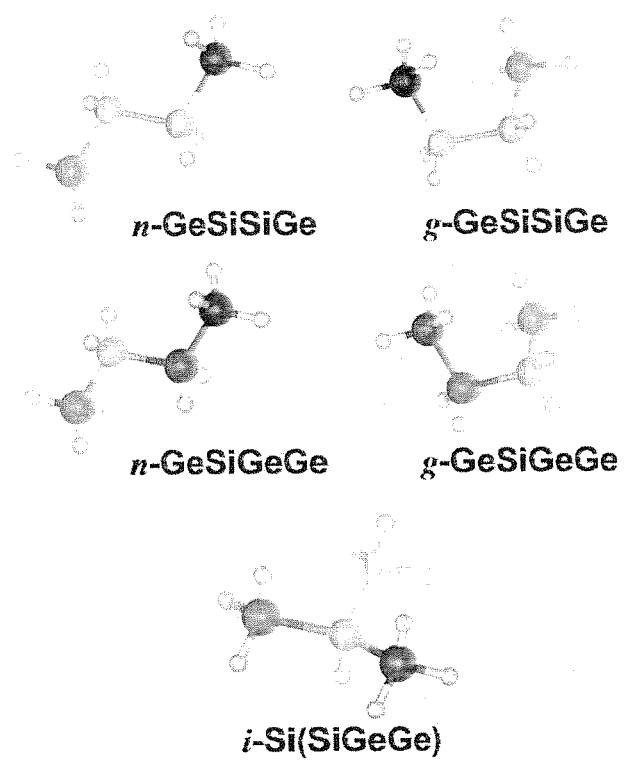
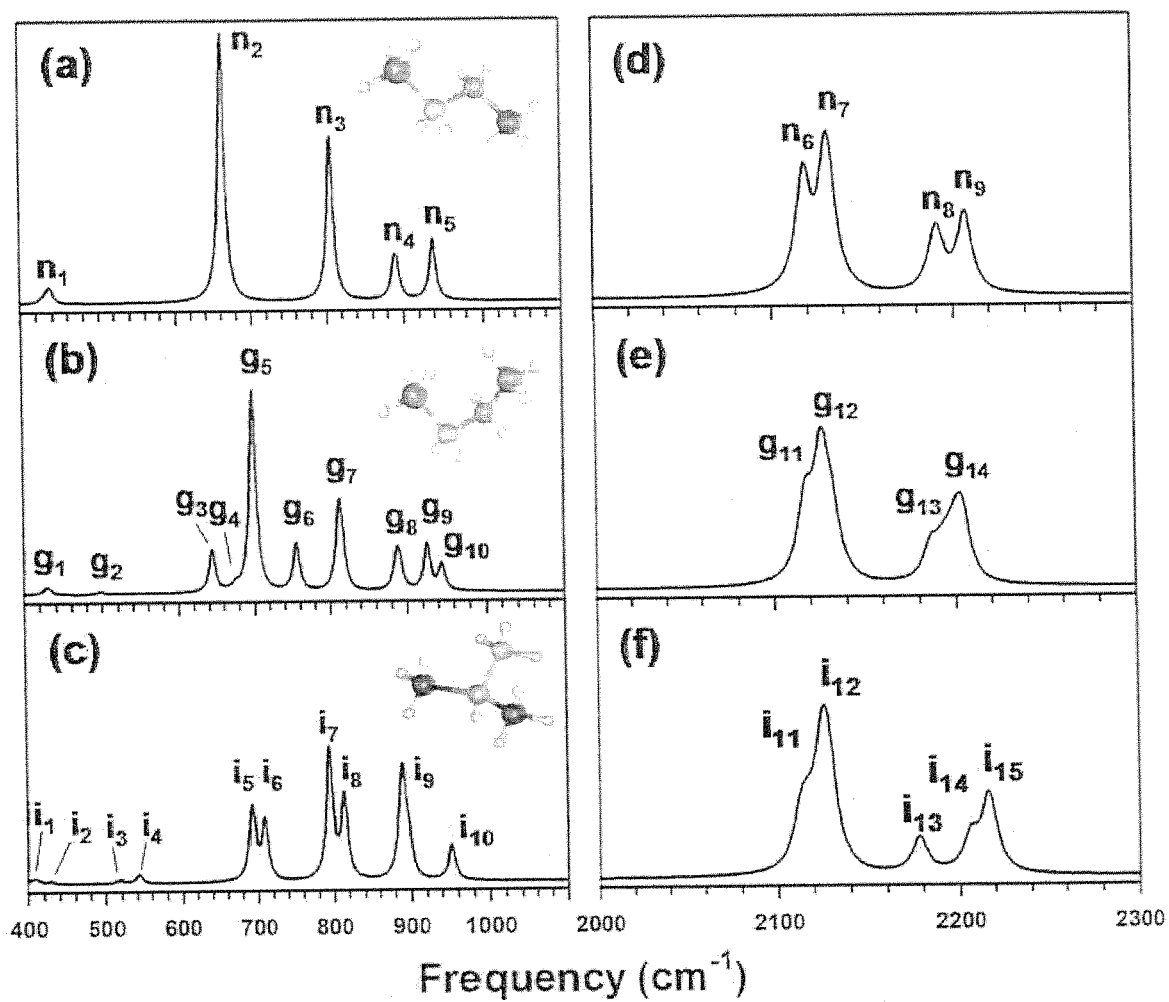


Figure 1

*Figure 2*

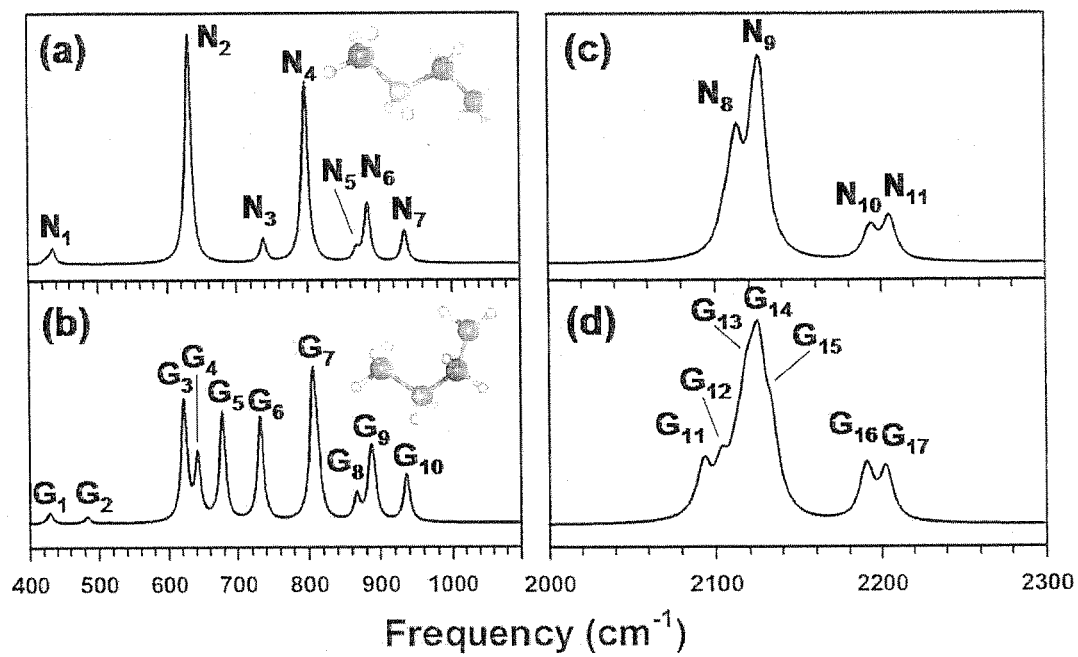


Figure 3

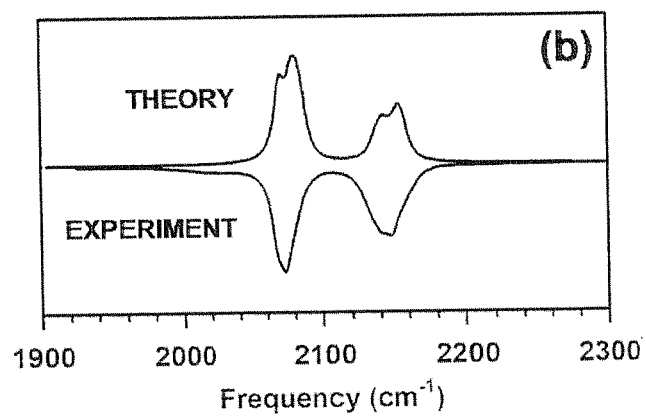
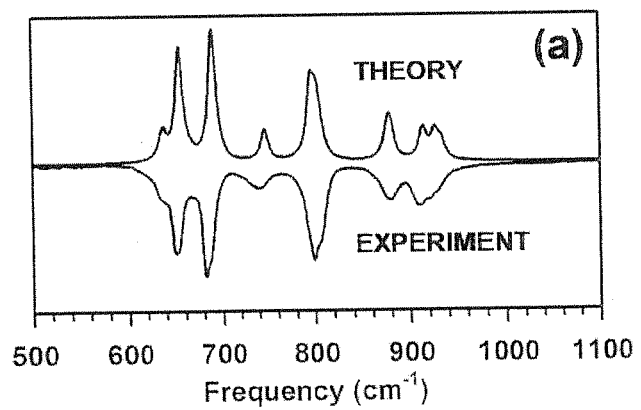


Figure 4

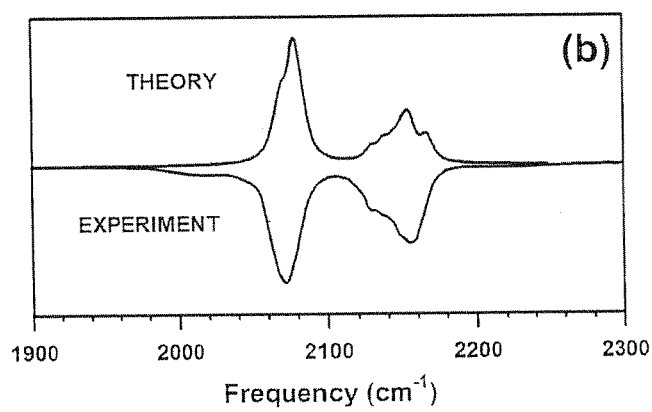
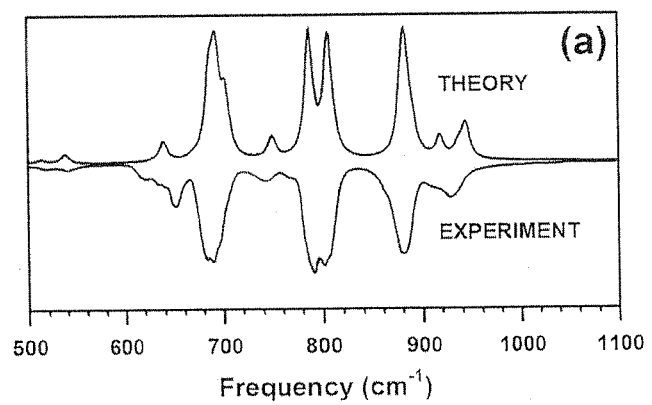


Figure 5

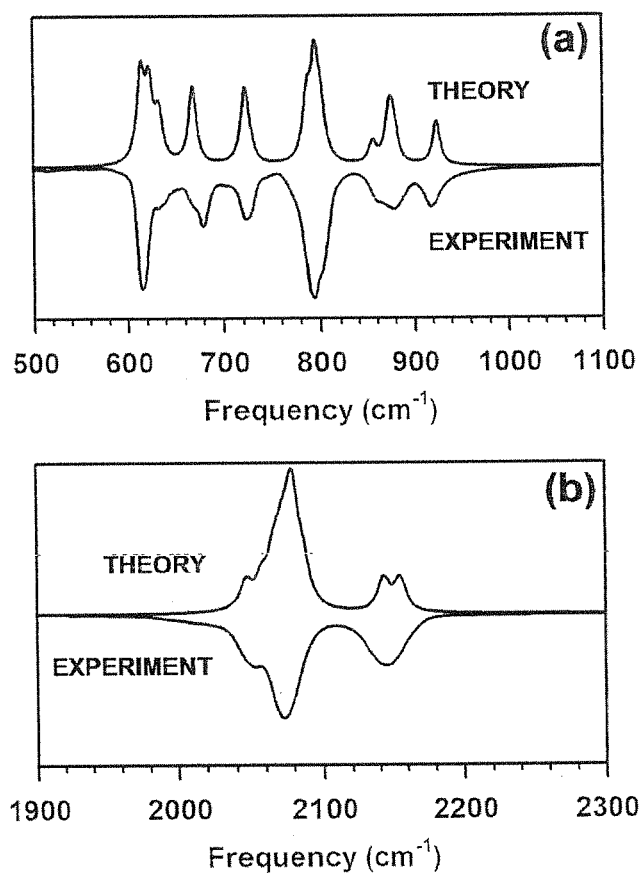


Figure 6

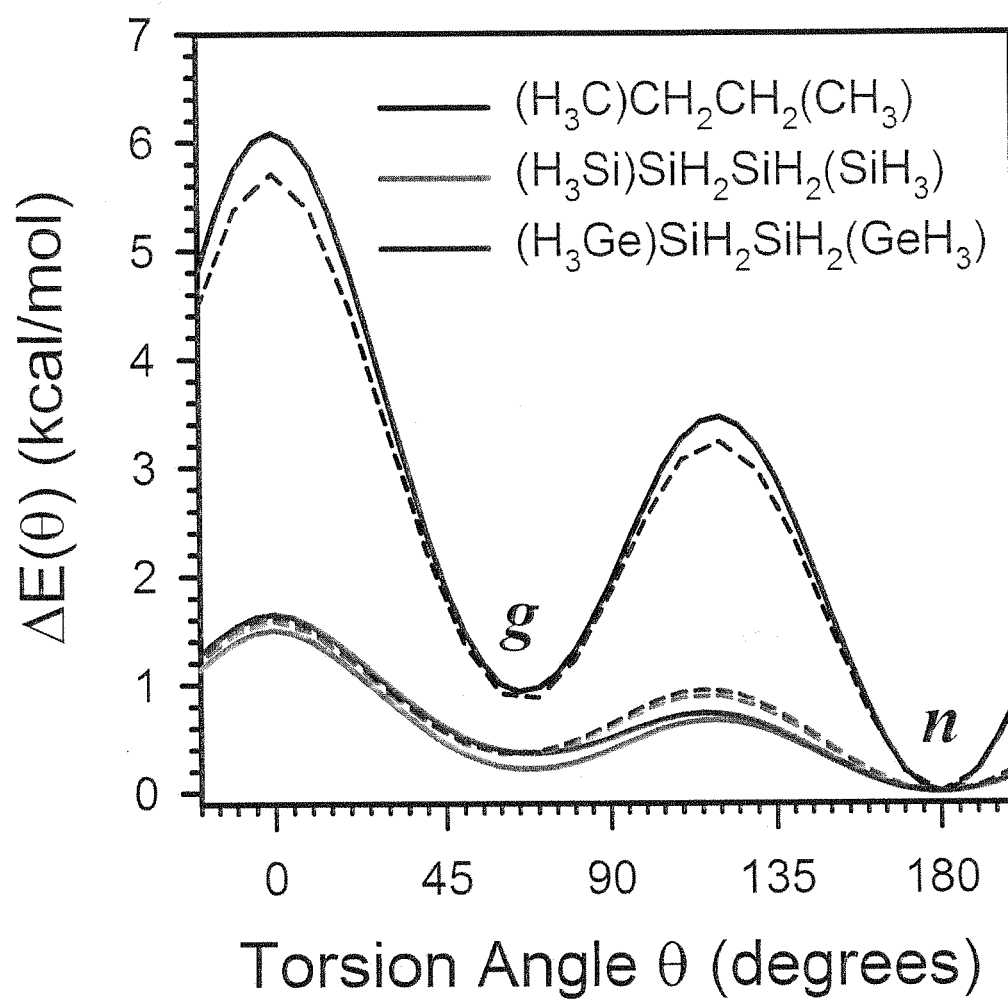
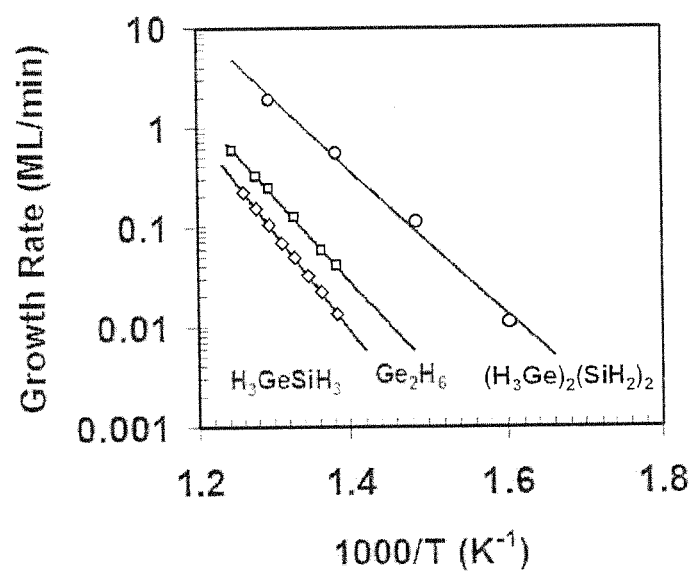


Figure 7

*Figure 8*

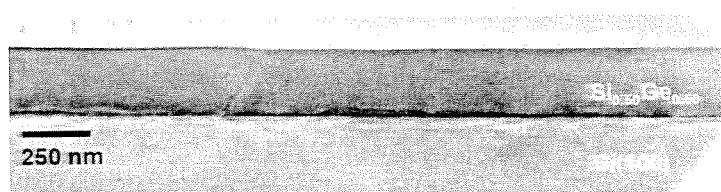


Figure 9

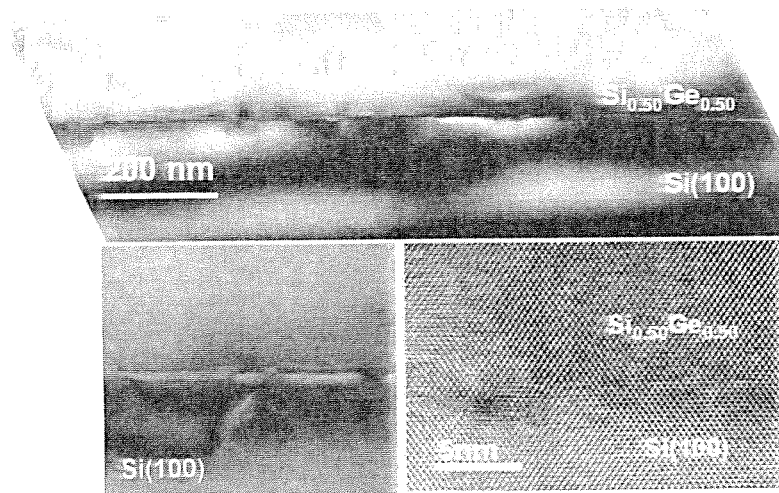


Figure 10

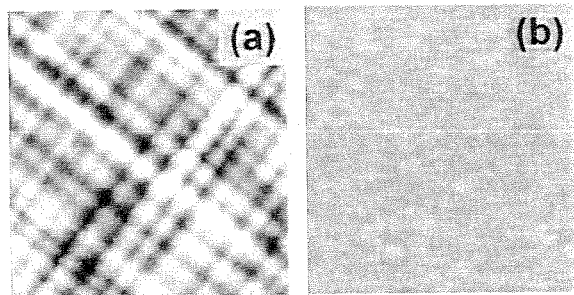


Figure 11

	<i>n</i> -GeSiSiGe	<i>g</i> -GeSiSiGe	<i>l</i> -GeSiGeGe	<i>n</i> -GeSiGeGe	<i>g</i> -GeSiGeGe
Bond lengths					
Si-Si	2.350	2.352	2.351		2.395, 2.400
Si-Ge	2.398	2.397	2.400	2.398	2.446
Ge-Ge				1.485	1.485
Si-H	1.485	1.486	1.488, 1.483		1.548, 1.542
Ge-H	1.539	1.538	1.539	1	
Bond angles					
Ge-Si-Ge			110.7		112.8
Si-Ge-Ge					113.4
Ge-Si-Si	112.6	112.8	111.2		107.8
H-Si-H	107.7	107.7	108.6		
H-Ge-H	108.3	108.2	108.3		109.0
H-Si-Ge	108.9	108.8	107.7	109.0, 109.2	109.3, 110.7
H-Ge-Si	110.5, 110.5, 111.0	110.7	108.4	109.5, 110.5, 111.1	
H-Si-Si					
Bond Torsions					
Ge-Si-Si-Ge	180.0	66.0	-33.1	180.0	64.1
Ge-Si-Ge-Ge				58.2, 62.0, 178.4	58.4, 61.7, 178.5
H-Ge-Ge-H				58.8, 61.4, 179.0	59.9, 60.1, 179.8
H-Ge-Si-H	58.6, 61.5, 178.8	58.5, 61.9, 178.9	53.1, 72.6, 179.7	58.8, 61.4, 179.0	58.7, 61.2, 178.8
H-Ge-Si-Ge			57.6, 62.2, 177.8	59.8, 59.8, 180.0	57.0, 174.5
H-Si-Ge-Ge			30.2	±58.6	
H-Ge-Si-Si	58.6, 61.5, 180.0	59.5, 60.4, 179.7	58.2, 61.8, 178.3		
Energetics					
E_0	-4739.094740	-4739.093652	-4739.094943	-6526.593697	-6526.593140
E_0+E_{ZPE}	-4739.013922	-4739.013009	-4739.014382	-6526.514649	-6526.513945
E_0+E_{rot}	-4739.003483	-4739.002561	-4739.003703	-6526.503627	-6526.503131
E_0+H_{corr}	-4739.002539	-4739.001616	-4739.002759	-6526.502683	-6526.502186
E_0+G_{corr}	-4739.051456	-4739.050695	-4739.052539	-6526.555562	-6526.553533

Figure 12

Sequence of macromolecular, polymeric units based on interconnected $(\text{GeH}_3)_2(\text{SiH}_2)_2$ monomers (a-d), en route to a diamond cubic Si-Ge lattice with concentration Ge_2Si_2 ($\text{Si}_{0.50}\text{Ge}_{0.50}$) (e). This material incorporates the Ge-Si-Si-Ge molecular core of $(\text{GeH}_3)_2(\text{SiH}_2)_2$ as the structural and compositional building block.

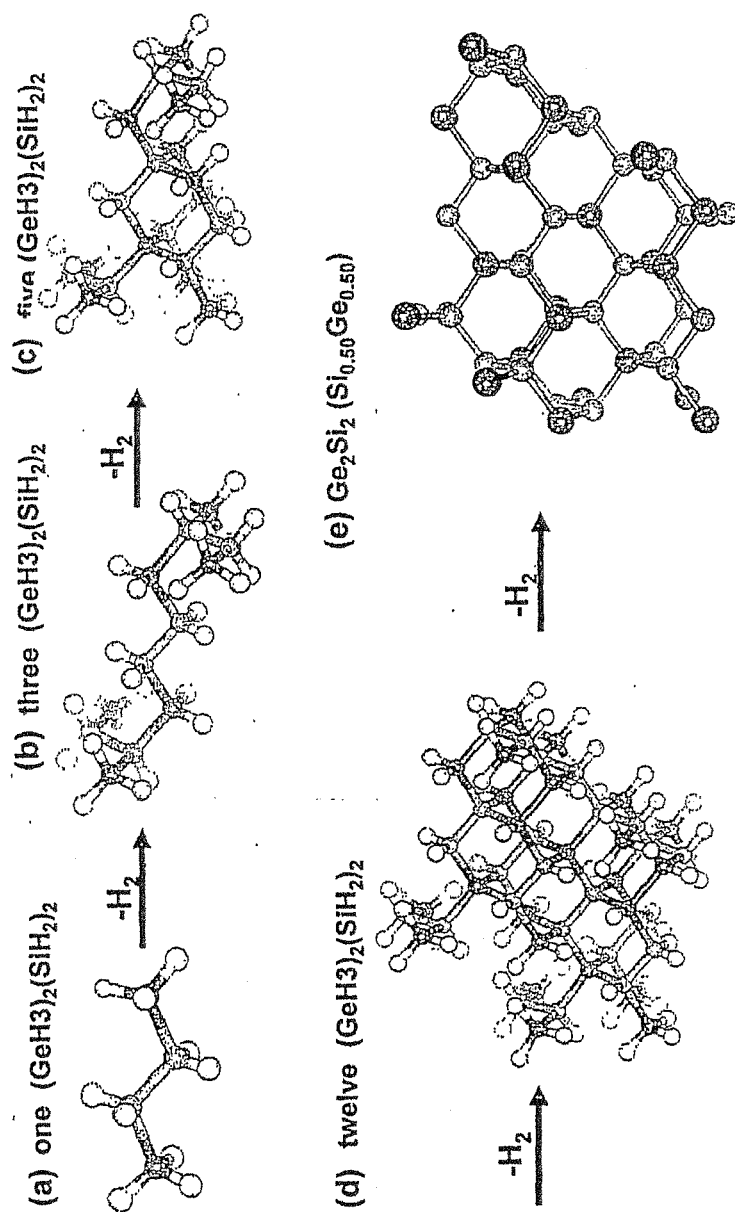


FIGURE 13A

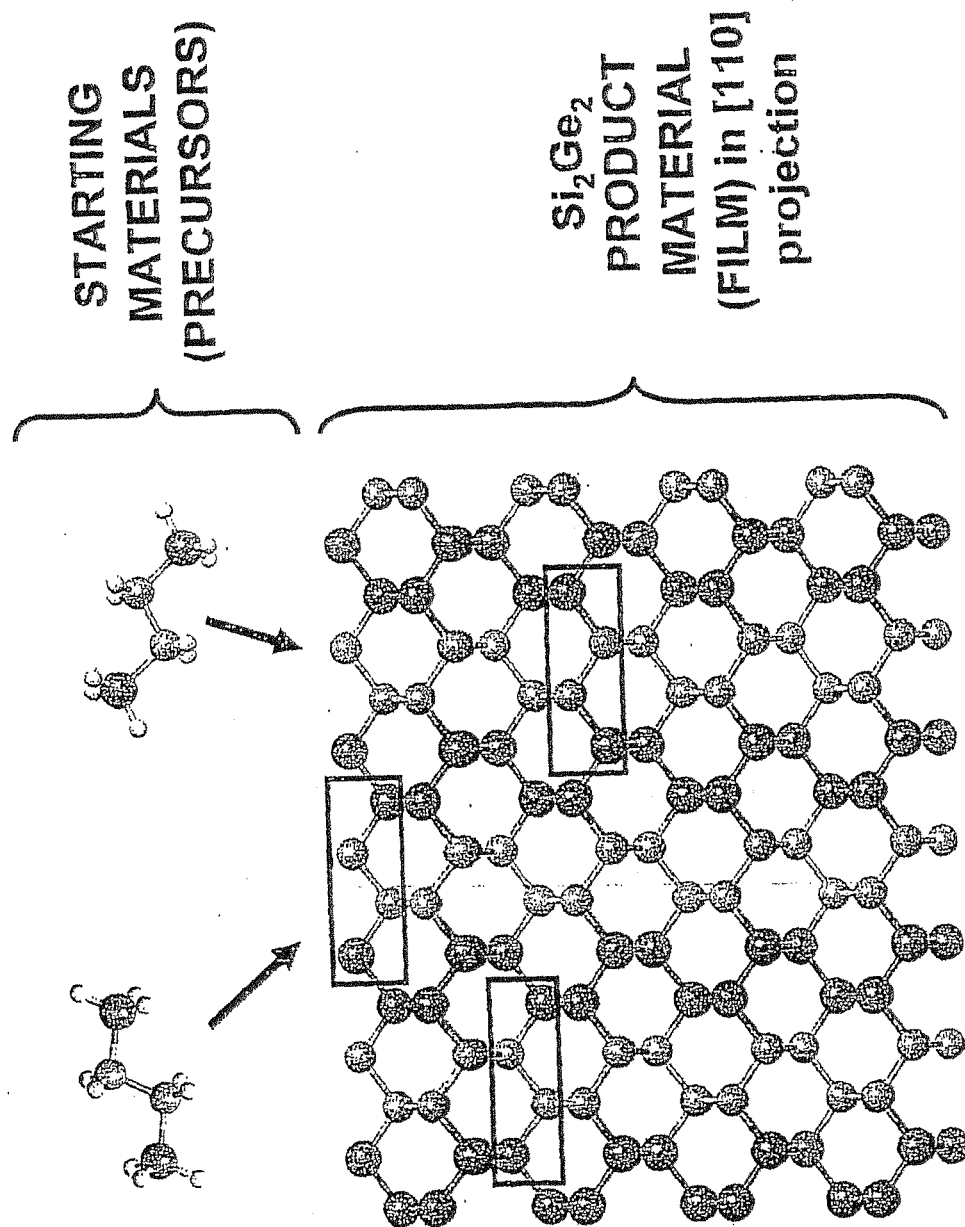


FIGURE 13B

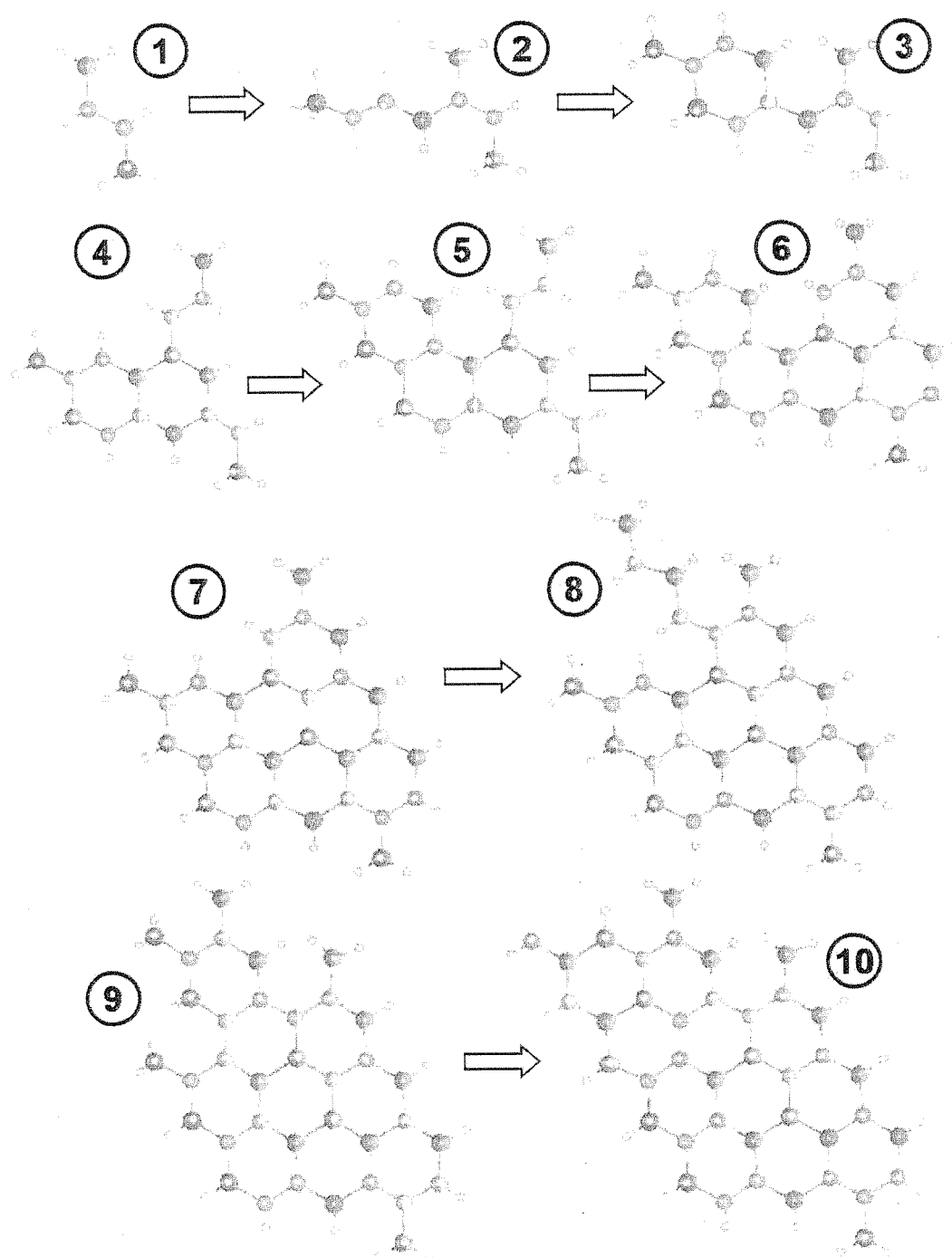


Figure 14

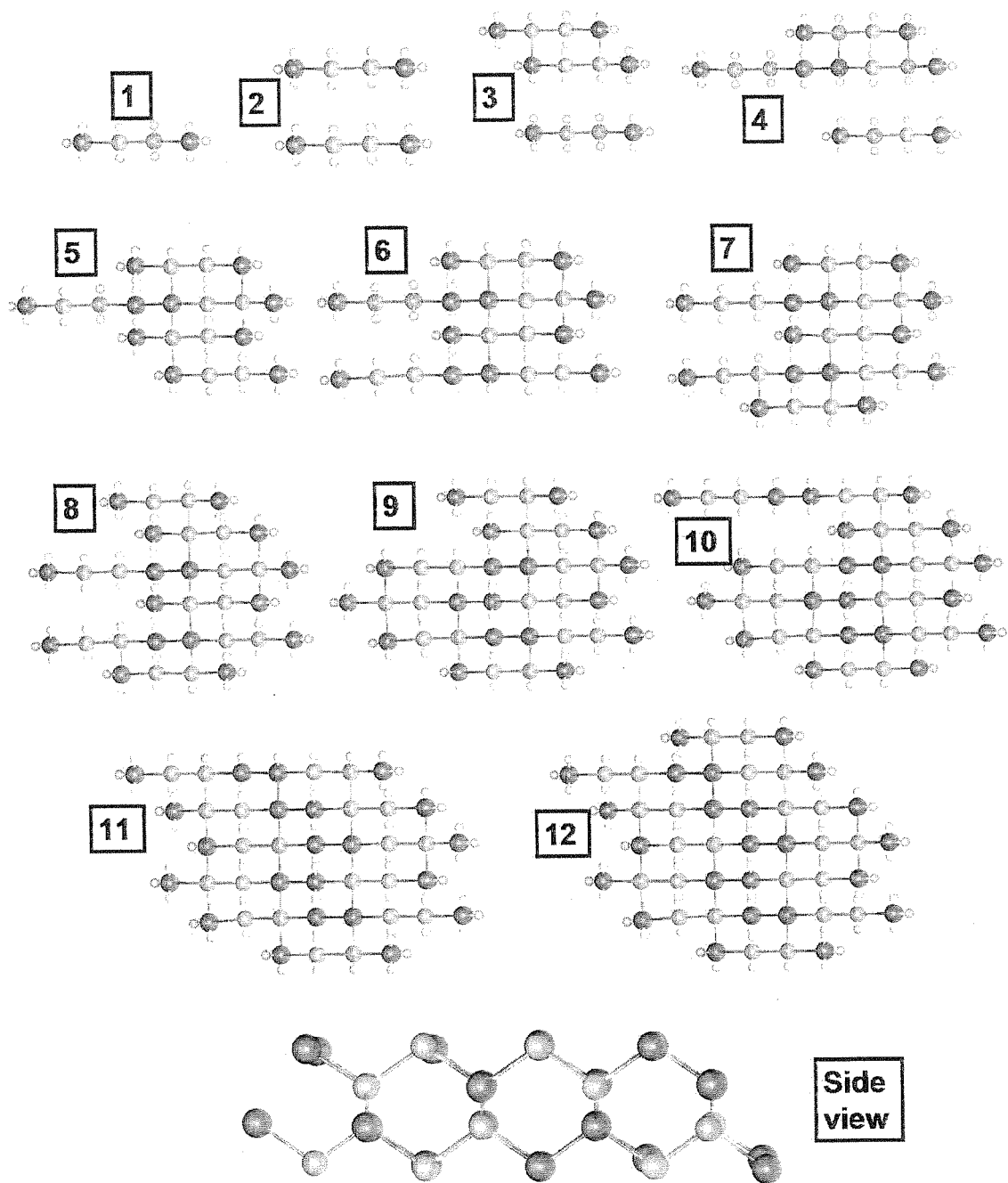


Figure 15