

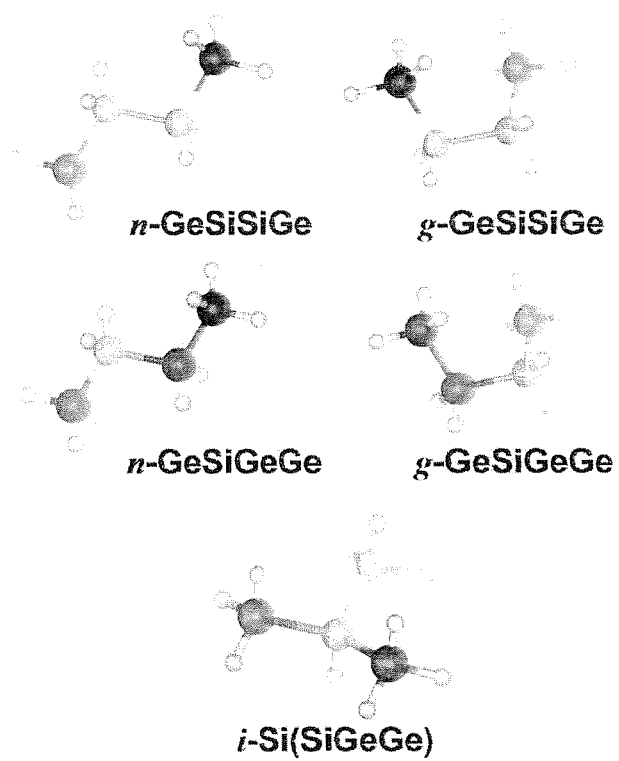


Figure 1

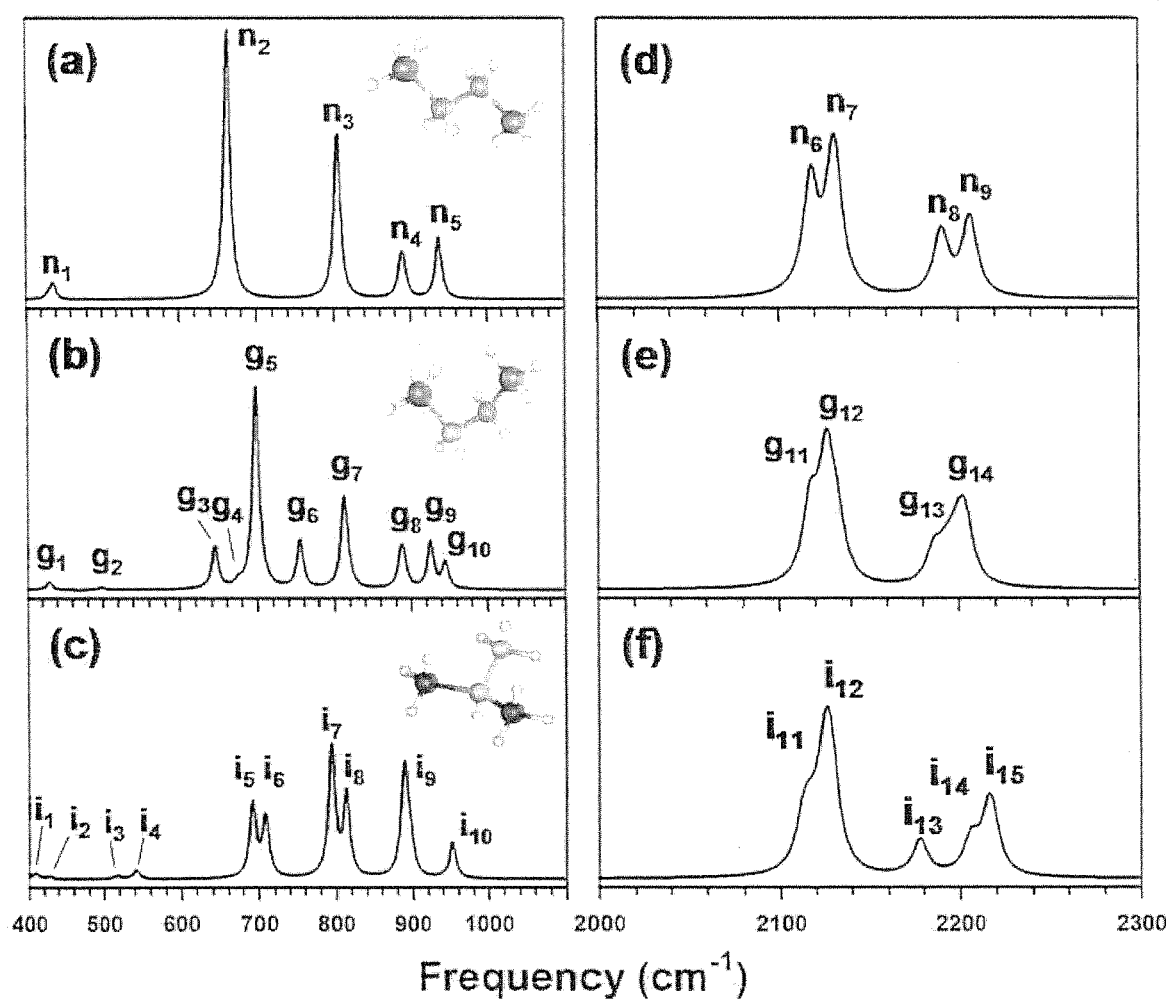


Figure 2

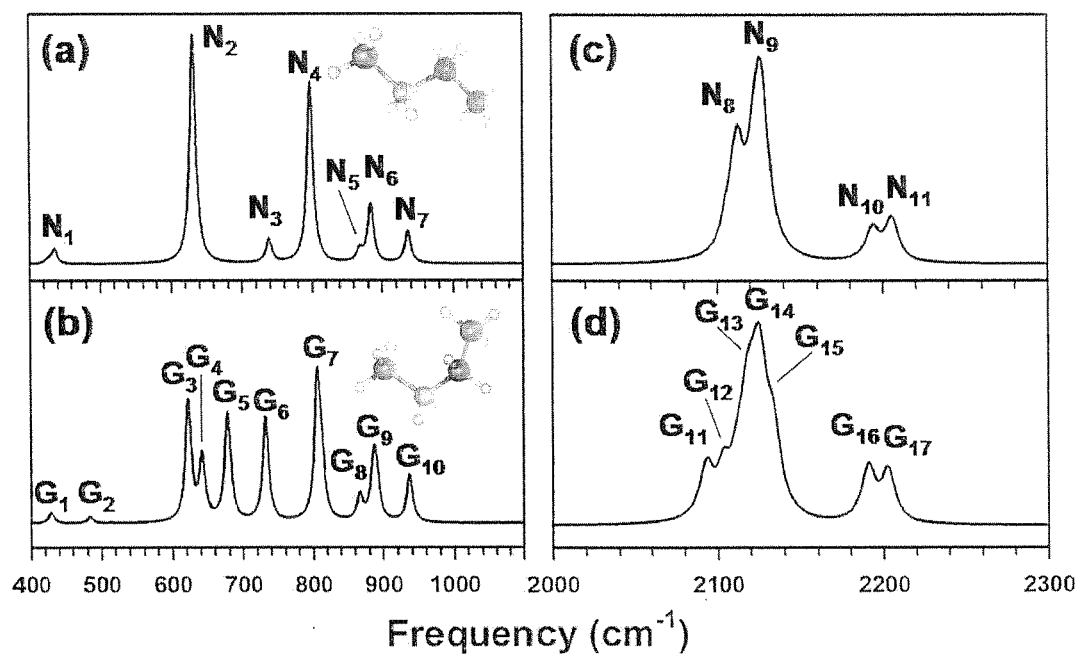


Figure 3

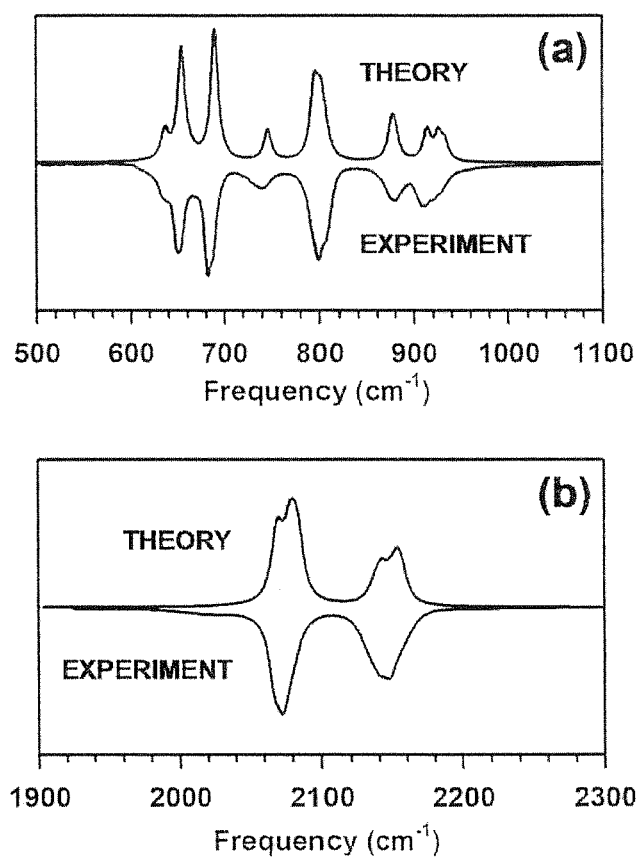


Figure 4

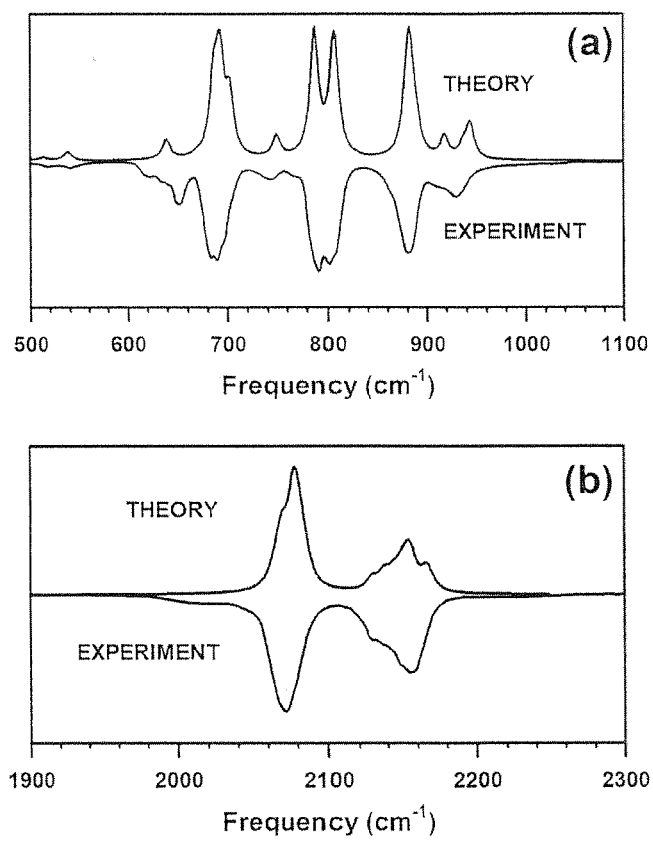


Figure 5

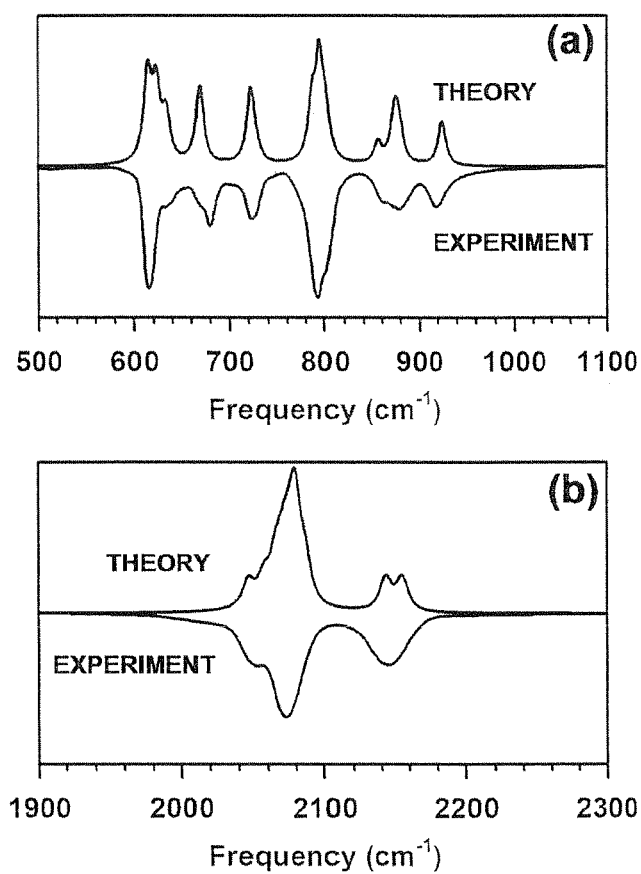


Figure 6

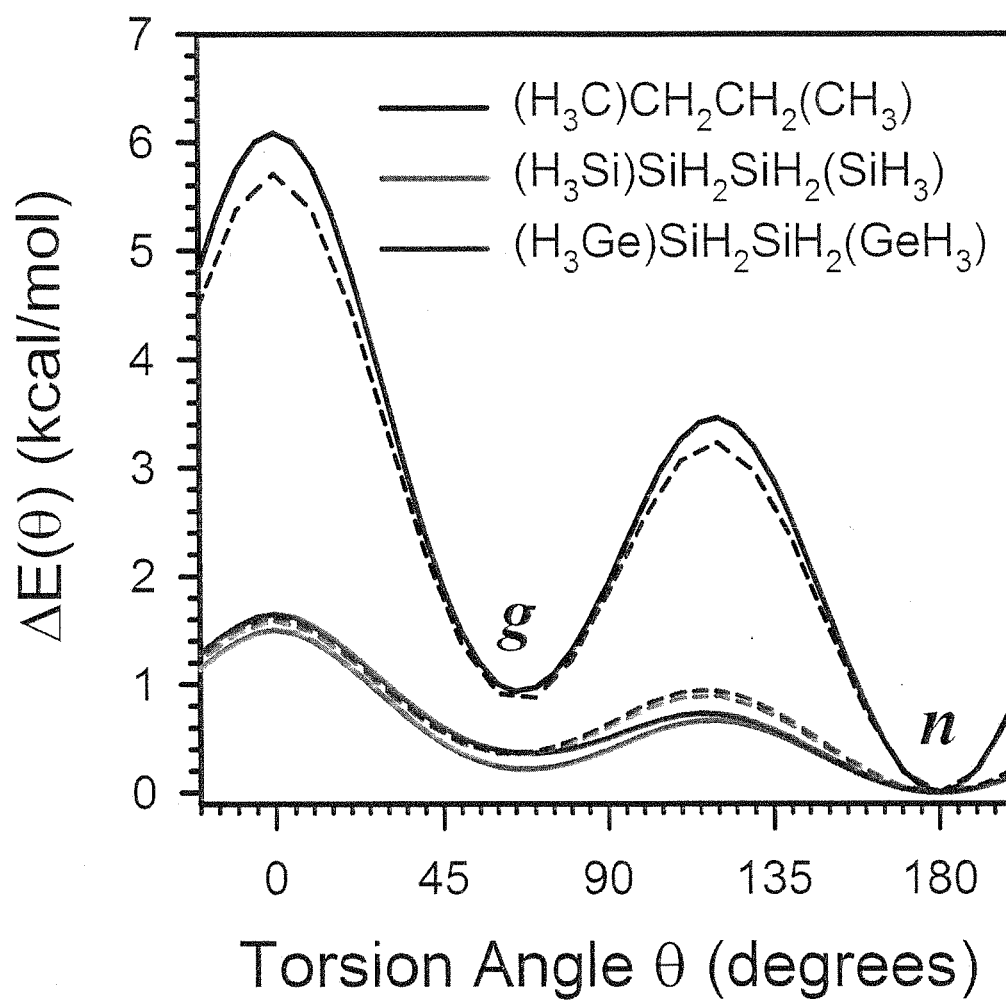


Figure 7

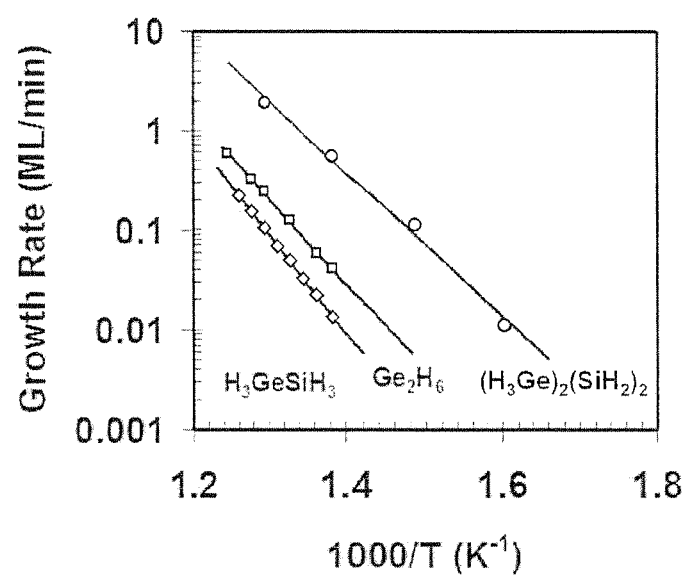


Figure 8



Figure 9

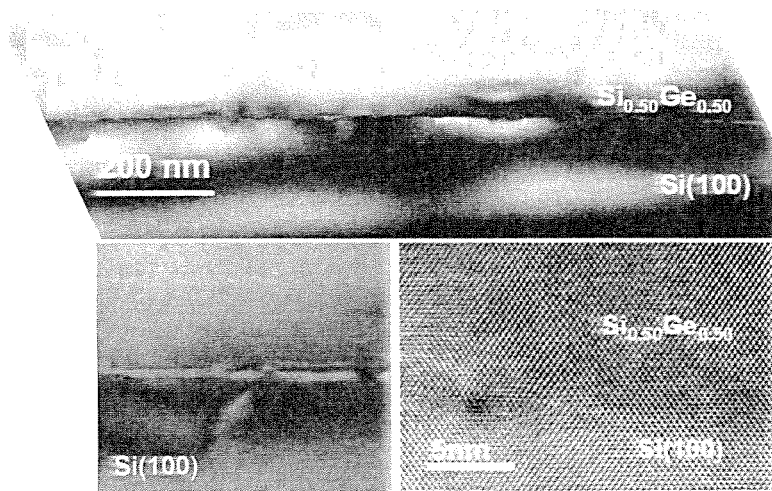


Figure 10

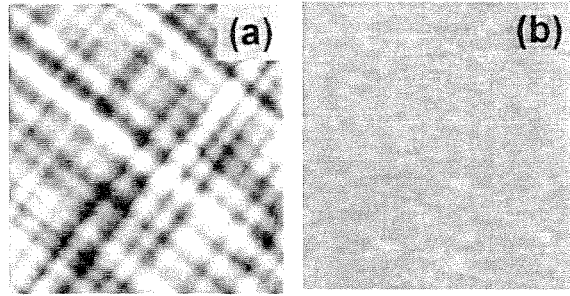


Figure 11

Bond lengths					
	<i>n</i> -GeSiSiGe	<i>g</i> -GeSiSiGe	<i>i</i> -GeSiGeGe	<i>n</i> -GeSiGeGe	<i>g</i> -GeSiGeGe
Si-Si	2.350	2.352	2.351		
Si-Ge	2.398	2.397	2.400	2.398	2.396, 2.400
Ge-Ge				2.446	2.446
Si-H	1.485	1.486	1.488, 1.483	1.485	1.485
Ge-H	1.539	1.538	1.539	1.548, 1.542	1.548, 1.542
Bond angles					
	<i>n</i> -GeSiSiGe	<i>g</i> -GeSiSiGe	<i>i</i> -GeSiGeGe	<i>n</i> -GeSiGeGe	<i>g</i> -GeSiGeGe
Ge-Si-Ge			110.7	112.7	112.8
Si-Ge-Ge				112.8	113.4
Ge-Si-Si	112.6	112.8	111.2		
H-Si-H	107.7	107.7	108.6	107.7	107.8
H-Ge-H	108.3	108.2	108.3		
H-Si-Ge	108.9	108.8	107.7	109.0, 109.2	109.0
H-Ge-Si	110.5, 110.5, 111.0	110.7		109.5, 110.5, 111.1	109.3, 110.7
H-Si-Si			108.4		
Bond Torsions					
	<i>n</i> -GeSiSiGe	<i>g</i> -GeSiSiGe	<i>i</i> -GeSiGeGe	<i>n</i> -GeSiGeGe	<i>g</i> -GeSiGeGe
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	59.8, 59.8, 180.0	58.7, 61.2, 178.8
H-Ge-Si-Ge			57.6, 62.2, 177.8	±58.6	57.0, 174.5
H-Si-Ge-Ge			30.2		
H-Ge-Si-Si	58.6, 61.5, 180.0	59.5, 60.4, 179.7	58.2, 61.8, 178.3		
Energetics					
	<i>n</i> -GeSiSiGe	<i>g</i> -GeSiSiGe	<i>i</i> -GeSiGeGe	<i>n</i> -GeSiGeGe	<i>g</i> -GeSiGeGe
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
$E_0 + E_{tot}$	-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

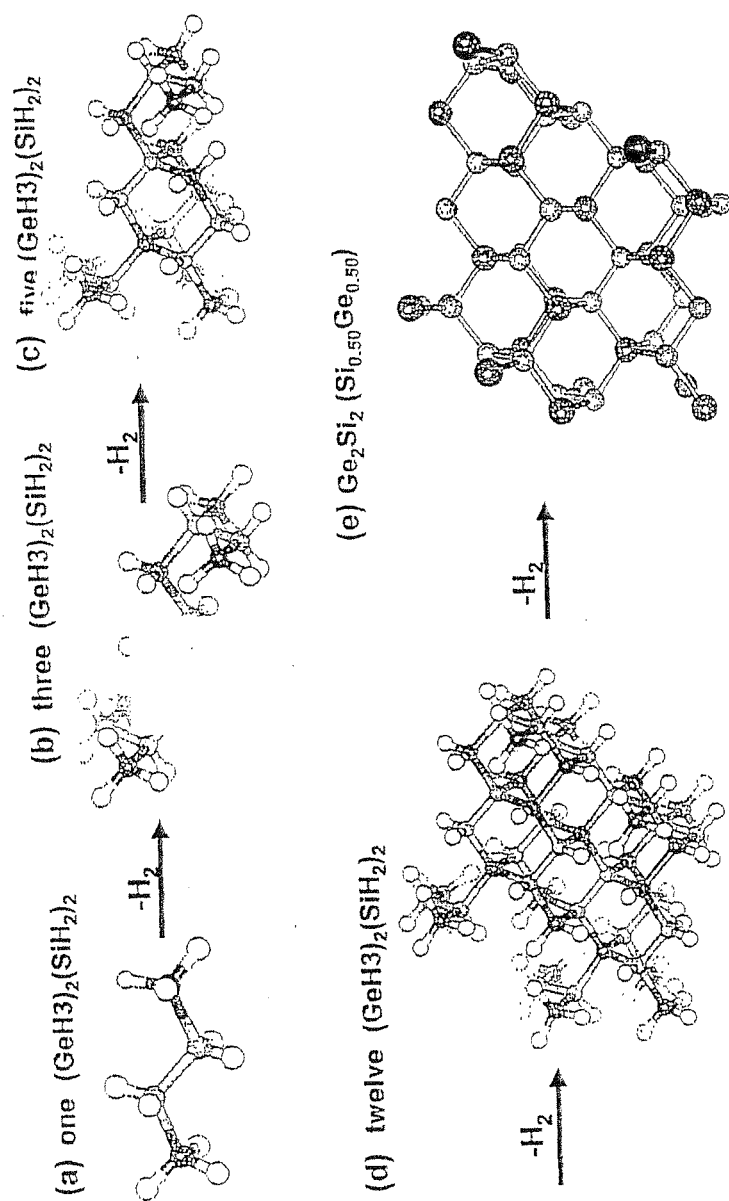
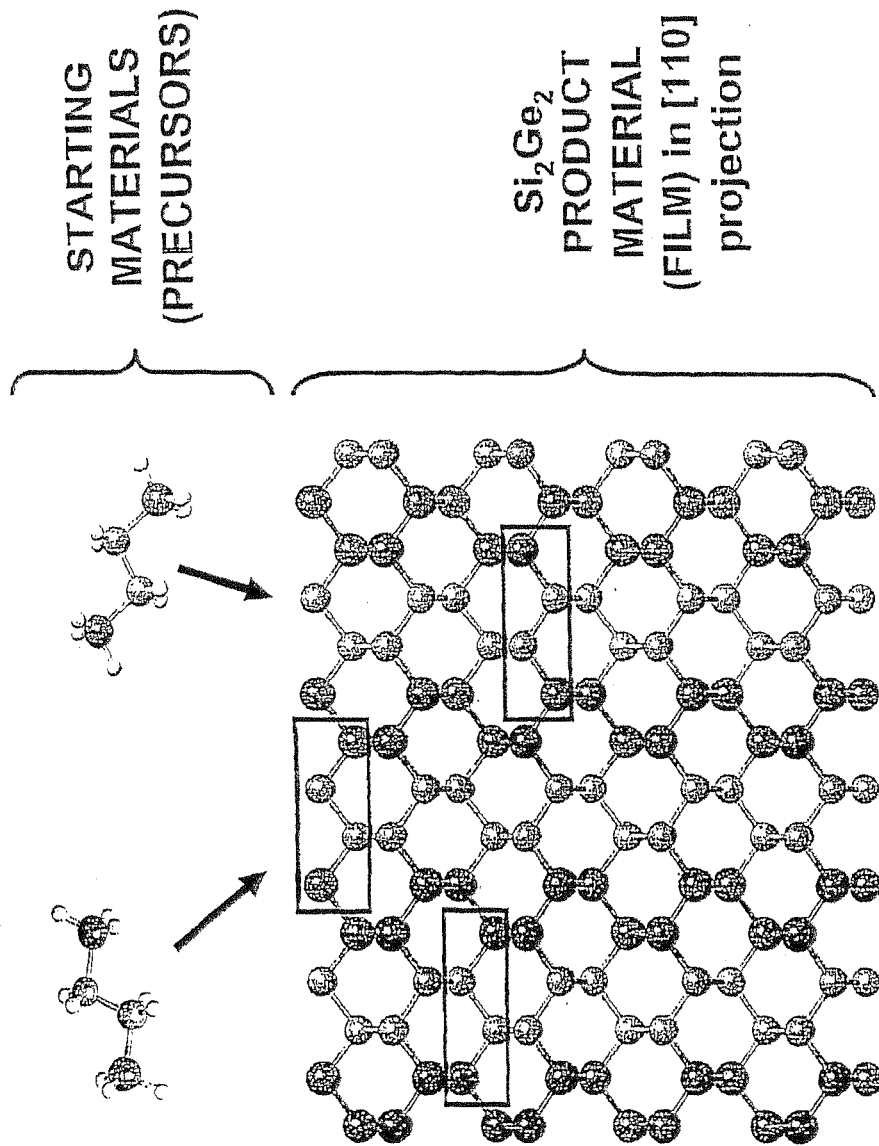


Figure 13A

*Figure 13B*

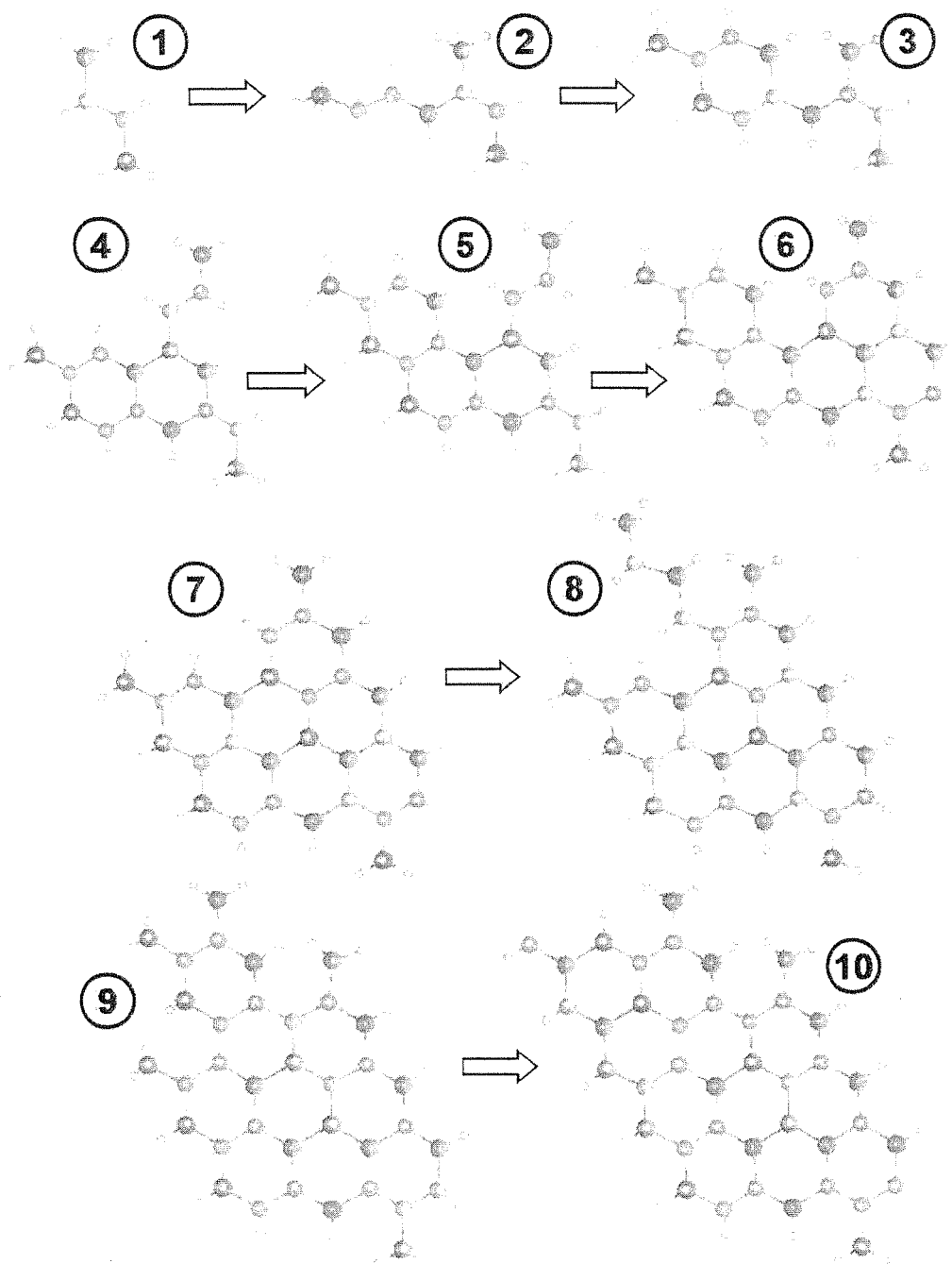


Figure 14

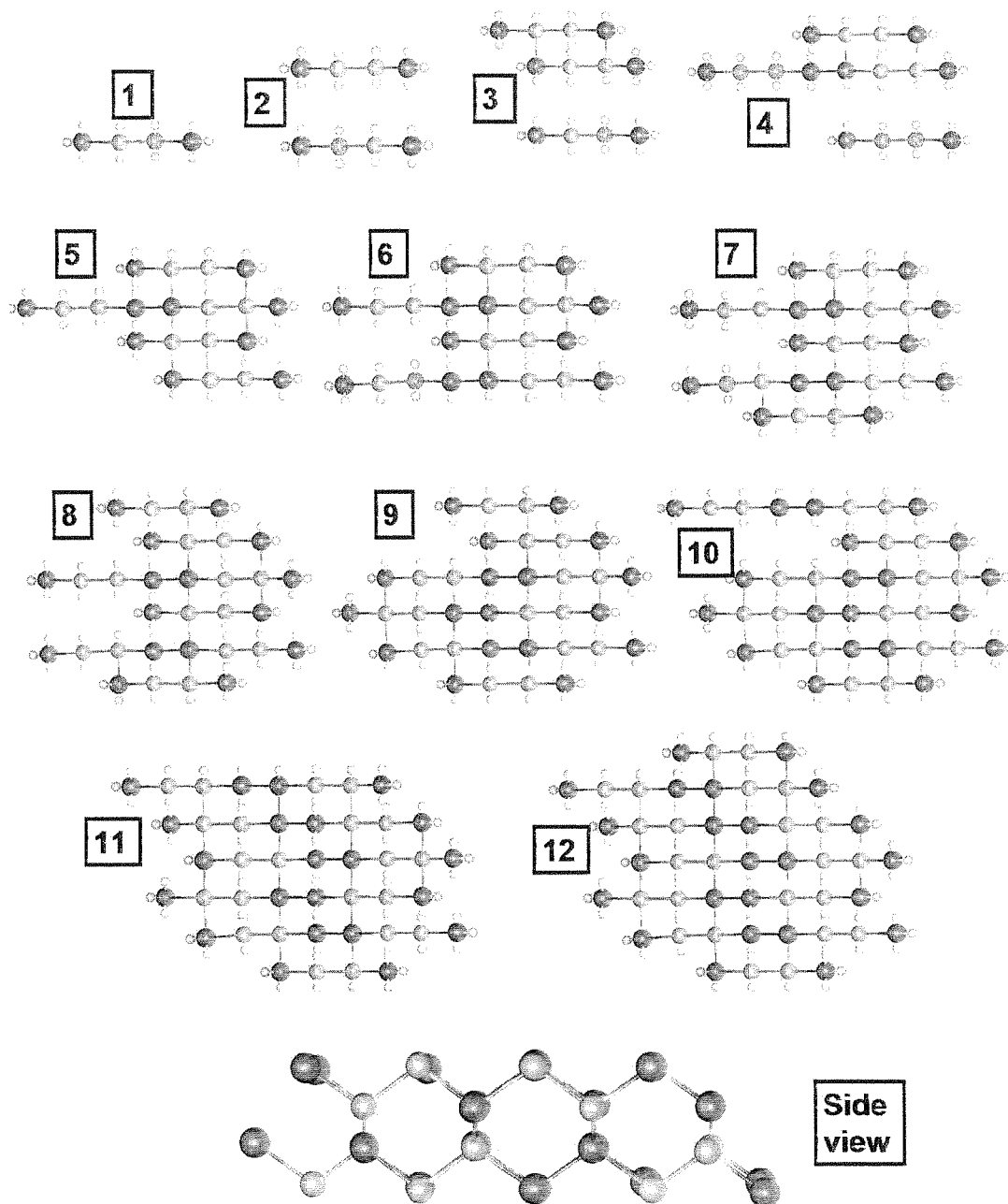


Figure 15