Post-anti-van't Hoff-Le Bel motif in atomically thin germanium-copper alloy film

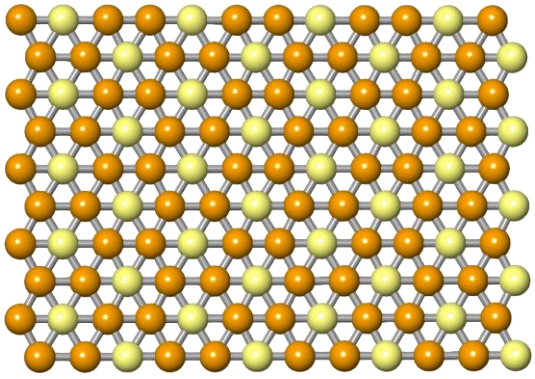
Supporting Information

Li-Ming Yang,*[1,2] Ivan A. Popov,[3] Alexander I. Boldyrev,[3] Thomas Heine,[2] Thomas Frauenheim,[1] and Eric Ganz[4]

[1]Bremen Center for Computational Materials Science, University of Bremen, Am Falturm 1, 28359, Bremen, Germany; [2]School of Eingineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany; [3]Department of Chemistry and Biochemistry, Utah State University, Logan, UT 84322, USA; [4]Department of Physics, University of Minnesota, 116 Church St., SE, Minneapolis, Minnesota 55416, USA. E-mail: lmyang.uio@gmail.com

The structural details (space group, lattice parameters, atomic coordinates) and relative energies of the optimized low-lying key isomers are given in VASP/POSCAR format.

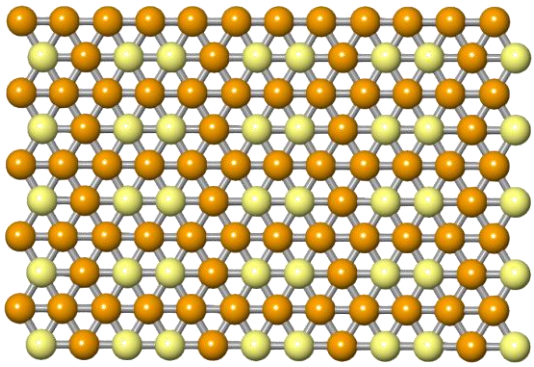
The optimization of crystal structures was performed *via* VASP code with Γ-centered Monkhorst-Pack (MP) K-points grid (sampling resolution $2\pi \times 0.0228$, for the ground state structure (isomer I), this sampling resolution corresponding to $12 \times 12 \times 1$ Kpoints). (The details of crystal structure optimization can be found in the section 2 **Computational details**)



Space group: *P6/mmm* (#191) relative energy: 0.00 meV

Lattice parameters: a = b = 4.21373 Å , c = 19.68492 Å (vacuum region), α = β = 90º, γ = 120º

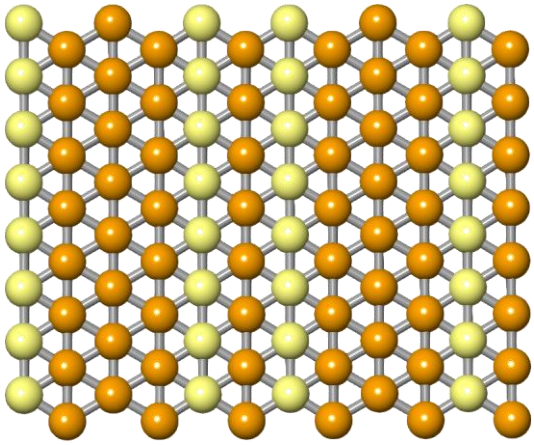
CONTCAR
1.00000000000000
4.2137296631329111 -0.0000592554142306 0.0000000000000000
-2.1069161482604906 3.6491673051941658 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.6849156944359684
Ge Cu
1 2
Direct
0.0000000000000000 0.0000000000000000 0.5000000000000000
0.3333417851259429 0.6666582438740560 0.5000000000000000
0.6666582438740560 0.3333417851259429 0.5000000000000000



Space group: *Pmmm* (#47) relative energy: 254.916 meV

Lattice parameters: a = 4.17142 Å , b = 19.70062 Å (vacuum region), c = 7.5129 Å , α = β = γ = 90º

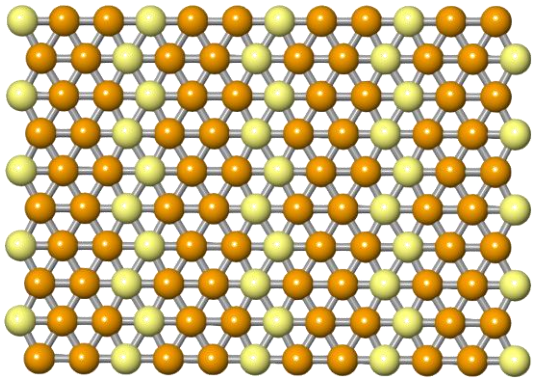
CONTCAR
1.00000000000000
4.1714175870926509 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.7006233835049009 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.5128982389434729
Cu Ge
4 2
Direct
0.2500000000000000 0.5000000000000000 0.7490237012551886
0.2500000000000000 0.5000000000000000 0.4176945965524362
0.2500000000000000 0.5000000000000000 0.0833058883403798
0.7500000000000000 0.5000000000000000 0.5832849263202065
0.7500000000000000 0.5000000000000000 0.2549241898991304
0.7500000000000000 0.5000000000000000 0.9117667056326592



Space group: *Pmmm* (#47) relative energy: 457.507 meV

Lattice parameters: a = 12.53171 Å , b = 14.74326 Å (vacuum region), c = 2.52093 Å , α = β = γ = 90º

CONTCAR
1.00000000000000
12.5317148178445894 0.0000000000000000 0.0000000000000008
0.0000000000000000 14.7432643619609092 0.0000000000000000
0.0000000000000000 0.0000000000000000 2.5209312829917110
Cu Ge
4 2
Direct
0.3327935887686526 0.5000000000000000 0.5000000000000000
0.6672063822313414 0.5000000000000000 0.5000000000000000
0.0000000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.1670664350549912 0.5000000000000000 0.0000000000000000
0.8329335649450089 0.5000000000000000 0.0000000000000000



Space group: *Pmma* (#51) relative energy: 502.176 meV

Lattice parameters: a = 4.37059 Å , b = 19.82528 Å (vacuum region), c = 7.35831 Å , α = β = γ = 90º

CONTCAR
1.00000000000000
4.3705906976017292 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8252800317059226 0.0000000000000000
-0.0000000000000002 0.0000000000000000 7.3583118714257987
Cu Ge
4 2
Direct
0.7500000000000000 0.5000000000000000 0.2483115308427558
0.2500000000000000 0.5000000000000000 0.7516884691572447
0.2500000000000000 0.5000000000000000 0.4211186799656181
0.7500000000000000 0.5000000000000000 0.5788813200343819
0.2500000000000000 0.5000000000000000 0.0943422601085344
0.7500000000000000 0.5000000000000000 0.9056577618914680