CHIN. PHYS. LETT. Vol. 37, No. 2 (2020) 026201

Stable Compositions, Structures and Electronic Properties in K–Ga Systems Under Pressure *

Chao Wang(王超), Yun-Xian Liu(刘云仙)**, Xin Chen(陈欣), Pin Lv(吕品),
Hai-Rui Sun(孙海瑞), Xiao-Bing Liu(刘晓兵)**

Laboratory of High Pressure Physics and Material Science, School of Physics and Physical Engineering, Qufu Normal University, Qufu 273165

(Received 21 October 2019)

New stable stoichiometries in K–Ga systems are firstly investigated up to 100 GPa by the unbiased structure searching techniques. Six novel compositions as K_4Ga, K_3Ga, K_2Ga, KGa, KGa_2 and KGa_4 are found to be thermodynamically stable under pressure. Most of the predicted stable phases exhibit metallic character, while the $Fd\bar{3}m$ KGa phase behaves as a semiconductor with a bandgap ∼1.62 eV. Notably, the gallium atoms exhibit different interesting morphologies; e.g., Ga_2 units, zigzag chains, six rings and cage. We further investigate the bonding nature of K–Ga systems with help of electron localization function and Bader charge analyses. Strong covalent bonding characteristics are found between the Ga and Ga atoms, and ionic bonding patterns are observed between the K and Ga atoms. Meanwhile, we notice charge transferring from the K atom to the Ga atom in the K–Ga systems. The present results can be helpful for understanding the diverse structures and properties of K–Ga binary compounds at high pressures.

PACS: 62.50.−p, 61.50.Ks, 71.20.−b DOI: 10.1088/0256-307X/37/2/026201

Nowadays, high-pressure science is an attractive and significant scientific research area, especially for material science. Under high pressure conditions, the crystal structure and physical properties of elements and materials can be changed effectively.[1–4] Consequently, novel compounds with unusual stoichiometries can be formed and stabilized, which may be quite different from the traditional chemical valence rules.[5–8] Recently, the pressure-induced potassium-X compounds (X denotes other elements) have attracted considerable attention because of their outstanding properties and growing applications in industry, such as unconventional stoichiometries, novel structures, superconductivity, high hardness or potential application as high performance battery materials and high-energy-density materials.[1–11]

In the K–Br and K–Cl systems, two (KBr_3 and KBr_5) and eight (K_3Cl, K_2Cl, K_3Cl_2, K_4Cl_3, K_5Cl_4, K_3Cl_5, KCl_3, and KCl_7) unconventional stoichiometric compounds have been experimentally synthesized and theoretically predicted at high pressures.[12,13] Using the Mao–Bell diamond anvil cell technology, three stoichiometric mixtures of KCu, KCu_2 and K_2Cu were discovered in potassium-copper mixtures.[14] A high pressure structure (anisotropic ω phase) as K_2Ag was found with graphite-like potassium layers.[15] The KC_8 and KP_2 compounds were predicted to be potential superconductors with $T_c = 0.14$ K and 22.01 K under pressure, respectively.[16,17] Furthermore, the KN_3 containing polymerized nitrogen under high pressure has also been extensively studied in experiment and theory because of its high potential application as a high energy density material.[18–20] Motivated by successful research on the diversity of phases and properties in the K–X systems under pressure, in this work, we carry systematic studies on inbinary K–Ga systems to explore the stable stoichiometries, structures, electronic properties and bonding patterns. We report that six novel compositions K_4Ga, K_3Ga, K_2Ga, KGa, KGa_2, and KGa_4 are found to be thermodynamically stable at pressures up to 100 GPa.

The stoichiometries and crystal structure prediction were performed using the evolutionary algorithm method as implemented in the USPEX code,[21–23] which has been successfully used in many systems.[24–29] Structures were produced randomly in the first generation with its population size of 20–60 structures. Every subsequent generation is produced from 60% of the lowest-enthalpy structures of the previous generation. New structures were produced by variation operator heredity (65% structures), atomic permutation (15%), and lattice mutation (20%). The calculation would keep working until the best structure contains more than 20 generations. The underlying *ab initio* structural relaxations, total energy, mechanical and electronic properties were calculated in the framework of density functional theory within the generalized gradient approximation Perdew–Burke–Ernzerhof (GGA-PBE)[30] exchange-correlation functional in the Vienna *ab initio* Simulation Package (VASP) code.[31] The all-electron projector augmented wave (PAW) method[32] with K $4s^1$ and Ga $4s^24p^1$ treated as the valence electrons. The plane-wave basis sets with the 400 eV cutoff, and dense Monkhorst–Pack meshes with $2\pi \times 0.03$ Å^{-1} were chosen to ensure that all of the enthalpy calculations are well converged to better than 1 meV/atom. To evaluate the electron localization and the electronic charge,

*Supported by the Shandong-Provincial Science Foundation (ZR2018PA010, ZR2017BA020, ZR2017BA012, ZR2019MA054 and 2019KJJ020), and the National Natural Science Foundation of China (11704220, 11674122, 11804184, 1180418 and 11974208).
**Corresponding author. Email: xiaobing.phy@qfnu.edu.cn; yunxianliu1988@163.com
© 2020 Chinese Physical Society and IOP Publishing Ltd

we used the electron localization function (ELF)[33] and Bader charge analysis.[34–36] The phonon calculations were carried out by supercell approach through the PHONOPY program.[37,38]

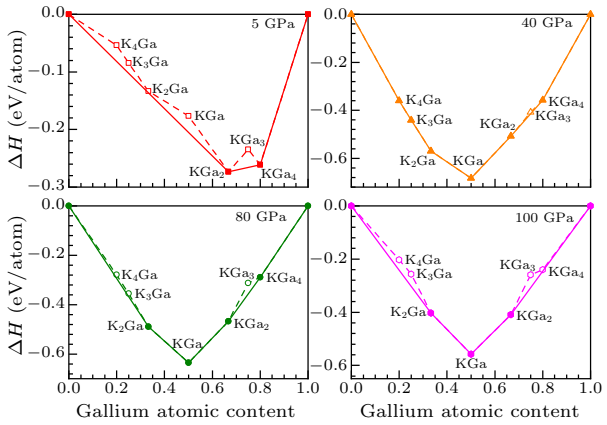

Fig. 1. Convex hull diagrams of the K–Ga systems at selected pressures of 5, 40, 80 and 100 GPa.

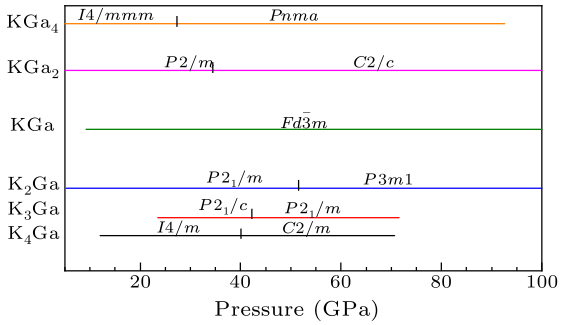

Fig. 2. Pressure–composition phase diagram of the K–Ga systems.

To study the thermodynamic stability of K–Ga compounds, we explore the crystal structures of various K_xGa_y ($x = y = 1, 2, 3, 4$) under high pressure up to 100 GPa. The calculated formation enthalpy values (ΔH_f) for the most stable candidate structures in the K–Ga systems are given in Fig. 1 and Fig. S1. The ΔH_f values are calculated for each stoichiometry with respect to the decomposition to elemental K and Ga, which can be expressed as

$$\Delta H_f(K_xGa_y) = [H(K_xGa_y) - xH(K) - yH(Ga)]/(x+y).$$

In general, new phases with their enthalpy values on the convex hull are stable against decomposition at a given pressure, while the structures above the convex hull are either metastable or unstable. We notice that the KGa_4 compound is the most thermodynamically stable composition throughout the entire studied pressure range. At 5 GPa, two stoichiometric KGa_2 and KGa_4 lie on the convex hull, demonstrating that they are energetically stable. Then, three more new stoichiometric K_4Ga, K_2Ga and KGa become stable at 20 GPa. At the pressure ranging from 40 and 60 GPa, a new stoichiometry appears on the hull as K_3Ga. With the exception of K_4Ga, K_3Ga and KGa_3 compounds, four stoichiometries (K_2Ga, KGa, KGa_2 and KGa_4) remain thermodynamically stable at 80 GPa. As pressures up to 100 GPa, only K_2Ga, KGa and KGa_2 are stable in our study.

The stable pressure ranges for the corresponding phases of K–Ga compounds are shown in Fig. 2. Moreover, Fig. S2 in the Supplementary Material gives the enthalpy curves for K_4Ga, K_3Ga, K_2Ga, KGa_2 and KGa_4. The morphologies of the predicted structures are presented in Figs. 3 and 4. It can be seen that K atoms exist in isolated form. For K_4Ga, a tetragonal phase $I4/m$ is preferred to be stable from 12 GPa to 40 GPa, then a monoclinic structure $C2/m$ becomes more favored till 70.7 GPa. In the $I4/m$ phase, Ga exists in atomic form, occupying the crystallographic $2a$ position, and K atoms lie the $8h$ position (Fig. 3(a)). For the $C2/m$ structure, Ga atoms form Ga_2 units with the distances of 2.68 Å (Fig. 3(b)). The stoichiometry of K_3Ga is predicted to be stable at 23.5 GPa, which has two monoclinic structures $P2_1/c$ and $P2_1/m$ with a phase transition pressure of 42.3 GPa. Ga atoms appear in the $P2_1/c$ structure as pairs and the Ga–Ga distance is 2.45 Å (Fig. 3(c)). In the $P2_1/m$ structure, Ga atoms form zigzag chains with the distance of 2.47 Å (Fig. 3(d)). For K_2Ga stoichiometry, a monoclinic structure $P2_1/m$ transforms into a trigonal phase $P\bar{3}m1$ at 51.5 GPa. In the $P2_1/m$, the Ga atoms are in the form of zigzag chains, the nearest Ga–Ga length is 2.58 Å (Fig. 3(e)). In the $P\bar{3}m1$ structure, the Ga atoms form six rings with the distance of 2.40 Å, in which the Ga atoms are not on the same plane (Fig. 3(f)).

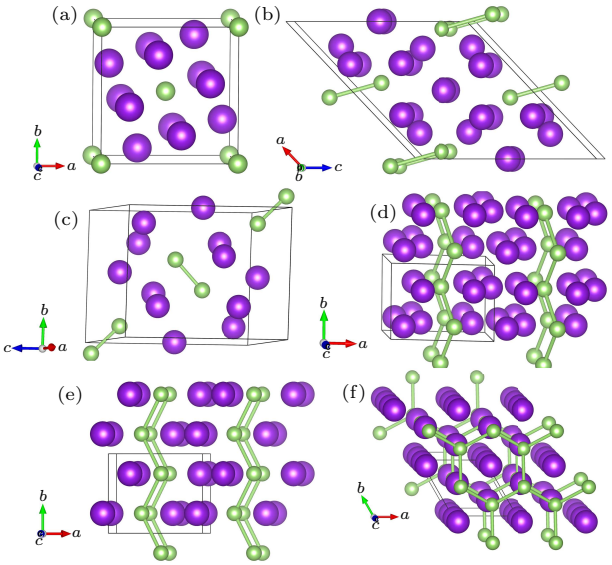

Fig. 3. Stable crystal structures of the predicted K-rich compounds: (a) $I4/m$ K_4Ga, (b) $C2/m$ K_4Ga, (c) $P2_1/c$ K_3Ga, (d) $P2_1/m$ K_3Ga, (e) $P2_1/m$ K_2Ga, and (f) $P\bar{3}m1$ K_2Ga. Purple and green balls denote K and Ga atoms, respectively.

Turning to KGa, we predict a cubic phase $Fd\bar{3}m$ with stable pressure range of 9.2–100 GPa. In the $Fd\bar{3}m$ structure, K and Ga atoms occupy the crystallographic $8a$ and $8b$ positions. Ga atoms form zigzag chains and the nearest distance is 2.53 Å, as displayed

in Fig. 4(a). For KGa_2, two monoclinic structures $P2/m$ and $C2/c$ are obtained at 20 and 60 GPa, and phase transition occurs at 34.5 GPa. For the $P2/m$ structure, there are two nonequivalent Ga atoms, in which one occupies the crystallographic $4o$ position and the other one sites at the crystallographic $2n$ position, forming eight rings with the nearest lengths of 2.50 Å (Fig. 4(b)). In the $C2/c$, Ga atoms constitute zigzag chains and the nearest lengths is 2.42 Å (Fig. 4(c)). For the KGa_4 composition, three structures of $I4/mmm$, $Pnma$ and $C2/m$ are predicted. The phase of $I4/mmm$ with the lowest enthalpy remains up to 27.3 GPa. For the Ga atoms, there are two nonequivalent positions, and they occupy the crystallographic $4e$ and $4d$ position, which form cages with the distance of 2.50 Å, as illustrated in Fig. 4(d). Then at higher pressure, $Pnma$ becomes more favored until 92.6 GPa, wherein Ga atoms occupy $4k$ and $2e$ positions, forming chains with the shortest Ga–Ga length of 2.33 Å (Fig. 4(e)). Table S1 in the Supplementary Material gives the detailed structural information for each phase of the K–Ga systems.

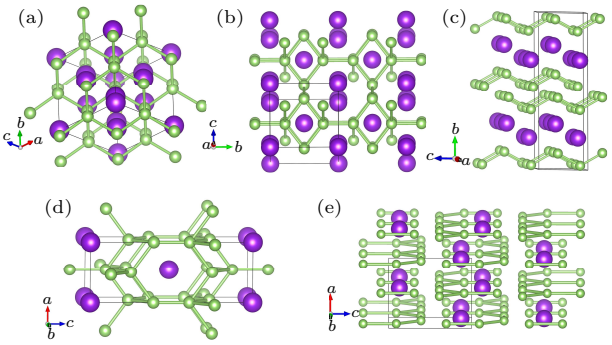

Fig. 4. Stable crystal structures of the predicted Ga-rich compounds: (a) $Fd\bar{3}m$ KGa, (b) $P2/m$ KGa_2, (c) $C2/c$ KGa_2, (d) $I4/mmm$ KGa_4, and (e) $Pnma$ KGa_4. Purple and green balls denote K and Ga atoms, respectively.

To judge their stability, the phonon dispersion curves for all the considered structures of K–Ga compounds are calculated, as presented in Fig. S3. No imaginary vibrational modes are observed in the Brillouin zone, suggesting that all the above phases are dynamically stable in their accessible pressures.

The electronic properties of various K–Ga compounds are also investigated by calculating band structures and the partial density of states (PDOS), as shown in Figs. 5 and 6 and Figs. S4–S7. Except the $Fd\bar{3}m$-KGa phase, all the other structures (K-rich: $I4/m$ K_4Ga, $C2/m$ K_4Ga, $P2_1/c$ K_3Ga, $P2_1/m$ K_3Ga, $P2_1/m$ K_2Ga, $P\bar{3}m1$ K_2Ga, Ga-rich: $P2/m$ KGa_2, $C2/c$ KGa_2, $I4/mmm$ KGa_4, $Pnma$ KGa_4) exhibit metallic feature by evidence of the finite electronic DOS at the Fermi level (Figs. 5 and 6). We notice different occupations of states near the Fermi level for K-rich and Ga-rich compounds. For K-rich compositions, the majority of occupied states near the Fermi level come from the K s, K p, K d and Ga p states (Fig. 5), whereas in Ga-rich phases, the Ga p states mainly occupy the Fermi level (Fig. 6). The structure $Fd\bar{3}m$ KGa is semiconductor with energy band gaps less than 3 eV, as depicted in Fig. S4.

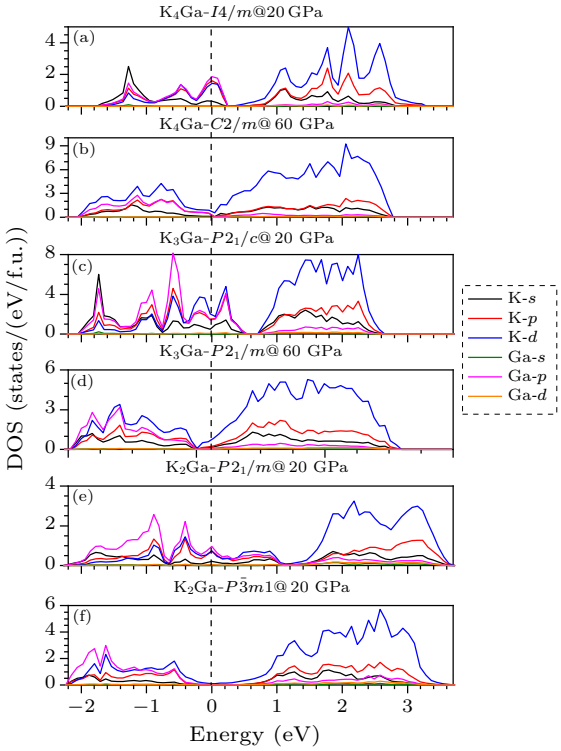

Fig. 5. Calculated PDOS of K-rich compounds. The vertical dashed line at zero is the Fermi level.

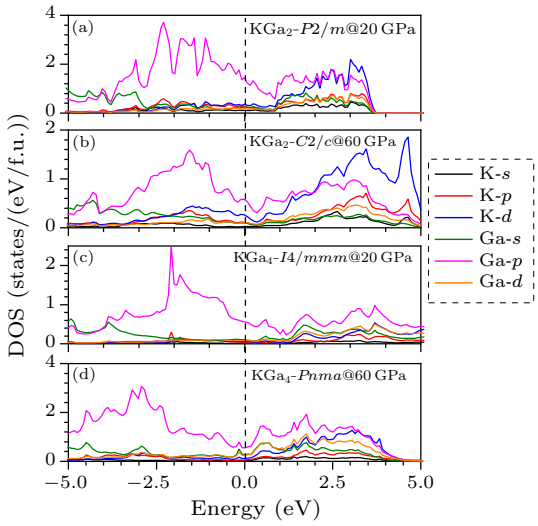

Fig. 6. Calculated PDOS of Ga-rich compounds. The vertical dashed line at zero is the Fermi level.

To further understand the bonding character of the K–Ga compounds, the electron localization function (ELF), a measure of relative electron localization in extended structures is calculated, as depicted in Fig. 7 and Figs. S8 and S9. Generally speaking, large ELF values (>0.5) occur in regions where there is a high tendency of electron pairing (such as cores, and lone pairs), indicating the formation of covalent bonds, while small values (<0.5) suggests non/less electron-localization, implying the existence of ionic/metallic

bonds between atoms. It is seen that the ELF values between Ga and Ga atoms are pretty high (∼0.7), which indicates a covalent bonding pattern, whereas there is no electron localization between K and Ga atoms, implying an ionic/metallic bonding character. Moreover, we also study the Charge transfer on the basis of the electron density using Bader analysis, as graphed in Table S2, which shows charge transfer from the K atom to Ga.

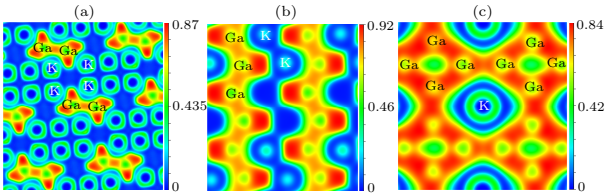

Fig. 7. ELFs of (a) $C2/m$ K_4Ga, (b) $P2_1/m$ K_2Ga, and (c) $P2/m$ KGa_2.

In summary, six unusual stoichiometries (K_4Ga, K_3Ga, K_2Ga, KGa, KGa_2 and KGa_4) of K–Ga compounds are discovered under high pressure using unbiased structure searching combined with density functional theory calculations. The predicted structures contain a rich variety of polygallium forms, such as Ga_2 units, zigzag chains, six rings (Ga_6 units) and cage. Electronic structure calculations suggest that the $Fd\bar{3}m$-KGa phase is semiconductor, while all the other predicted K–Ga systems exhibit metallic character. Further analysis of the bonding nature shows that charges transfer from potassium atoms to gallium atoms. Our results are important for understanding the structures and properties of potassium-gallium under high pressure.

The calculations were performed at the High Performance Computing Center (HPCC) of Qufu Normal University.

References

[1] Ma Y, Eremets M and Oganov A R 2009 *Nature* **458** 182
[2] Liu M, Tian C and Huang X 2019 *Chin. Phys. B* **28** 068101
[3] Duan D, Liu Y and Tian F 2015 *Sci. Rep.* **4** 6968
[4] Jia Y T, Zhao J F and Zhang S J 2019 *Chin. Phys. Lett.* **36** 087401
[5] Lin J, Zhang S and Guan W 2018 *J. Am. Chem. Soc.* **140** 9545
[6] Li P, Cui W and Li R 2017 *Chin. Phys. Lett.* **34** 076201
[7] Li Y, Feng X and Liu H 2018 *Nat. Commun.* **9** 722
[8] Sun G, Huang H and Li Y 2016 *Chin. Phys. Lett.* **33** 026104
[9] Li Q, Zhou D and Zheng W 2013 *Phys. Rev. Lett.* **110** 136403
[10] Lu C, Li Q and Ma Y 2017 *Phys. Rev. Lett.* **119** 115503
[11] McCulloch W D, Ren X and Yu M 2015 *ACS Appl. Mater. & Interfaces* **7** 26158
[12] Patel N N, Verma A K and Mishra A K 2017 *Phys. Chem. Chem. Phys.* **19** 7996
[13] Zhang W, Oganov A R and Zhu Q 2016 *Sci. Rep.* **6** 26265
[14] Snider T S and Badding J V 2004 *Solid State Commun.* **131** 157
[15] Atou T, Hasegawa M and Parker L 1996 *J. Am. Chem. Soc.* **118** 12104
[16] Xue M, Chen G and Yang H 2012 *J. Am. Chem. Soc.* **134** 6536
[17] Liu Y, Wang C and Kong X 2017 *Inorg. Chem.* **56** 12529
[18] Ji C, Zhang F and Hou D 2011 *J. Phys. Chem. Solids* **72** 736
[19] Li J, Wang X and Xu N 2013 *Europhys. Lett.* **104** 16005
[20] Zhang M, Yan H and Wei Q 2015 *RSC Adv.* **5** 11825
[21] Oganov A R and Glass C W 2006 *J. Chem. Phys.* **124** 244704
[22] Oganov A R, Lyakhov A O and Valle M 2011 *Acc. Chem. Res.* **44** 227
[23] Lyakhov A O, Oganov A R and Stokes H T 2013 *Comput. Phys. Commun.* **184** 1172
[24] Zhang H, Hu C and Wang D 2018 *Chin. Phys. B* **27** 083601
[25] Liu Y, Wang C and Lv P 2018 *Solid State Commun.* **280** 18
[26] Wang Y, Tian F and Li D 2019 *Chin. Phys. B* **28** 056104
[27] Wang C, Liu Y, Lv P 2018 *Chem. Eur. J.* **24** 18757
[28] Chu B, Zhao Y and Yan J 2018 *Chin. Phys. Lett.* **35** 016401
[29] Li Q, Wang Z and Yu Y 2019 *Chin. Phys. B* **28** 013101
[30] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[31] Kresse G and Furthmüller J 1996 *Comput. Mater. Sci.* **6** 15
[32] Kresse G and Joubert D 1999 *Phys. Rev. B* **59** 1758
[33] Becke A D and Edgecombe K E 1990 *J. Chem. Phys.* **92** 5397
[34] Bader R F 1985 *Acc. Chem. Res.* **18** 9
[35] Henkelman G, Arnaldsson A and Jónsson H 2006 *Comput. Mater. Sci.* **36** 354
[36] Tang W, Sanville E and Henkelman G 2009 *J. Phys.: Condens. Matter* **21** 084204
[37] Parlinski K, Li Z and Kawazoe Y 1997 *Phys. Rev. Lett.* **78** 4063
[38] Togo A, Oba F and Tanaka I 2008 *Phys. Rev. B* **78** 134106

Supplementary Material: Stable compositions, Structures and Electronic Properties in K–Ga Systems under Pressure *

Chao Wang(王超), Yunxian Liu(刘云仙)**, Xin Chen(陈欣), Pin Lv(吕品), Hairui Sun(孙海瑞), Xiaobing Liu(刘晓兵)**

Laboratory of High Pressure Physics and Material Science, School of Physics and Physical Engineering, Qufu Normal University, Qufu, 273165, P. R. China

**Email: xiaobing.phy@qfnu.edu.cn; yunxianliu1988@163.com

Figure S1: Convex hull diagrams of the K−Ga system at 20 and 60 GPa.

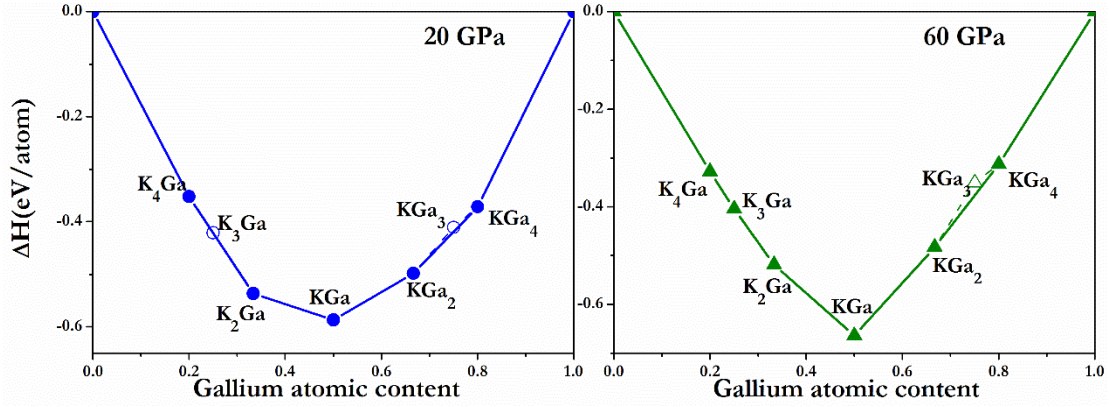

Figure S2: Enthalpy curves for K_4Ga, K_3Ga, K_2Ga, KGa_2 and KGa_4.

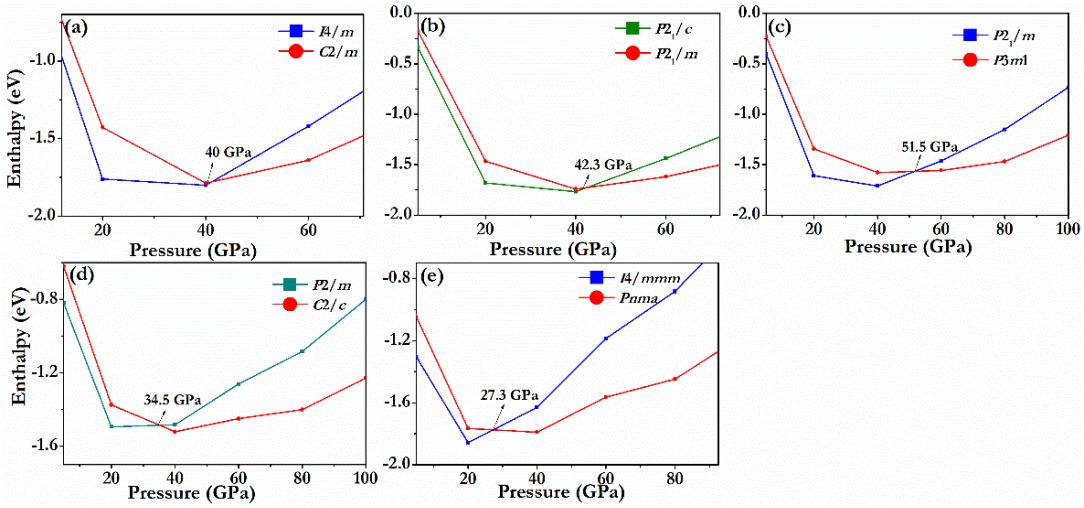

Figure S3: Phonon dispersion curves for K−Ga compounds at different pressures.

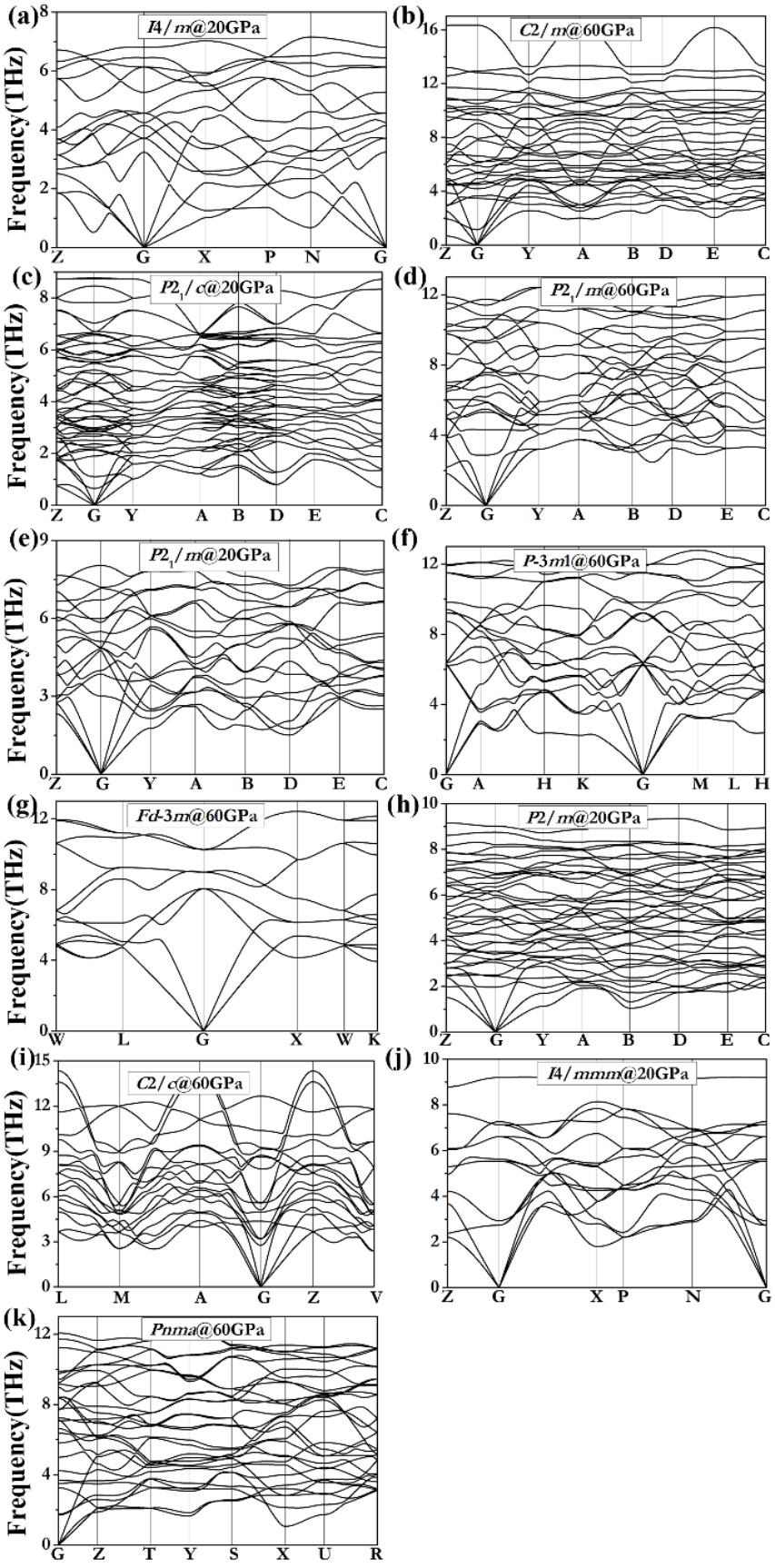

Figure S4: Calculated partial density of states (PDOS) of *Fd*-3*m*-KGa.

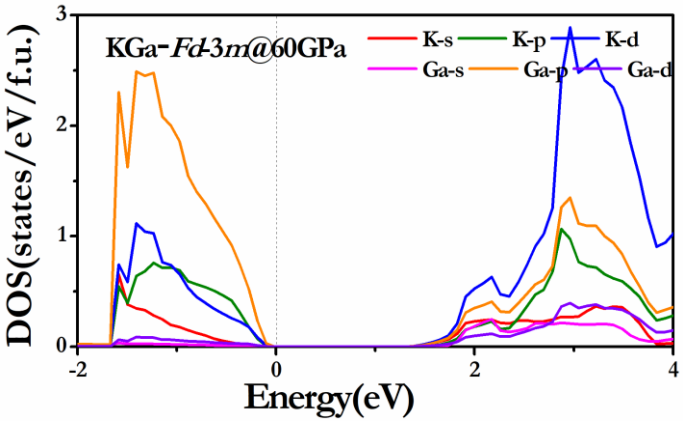

Figure S5: Calculated band structures of K-rich compounds: (a)*I*4/*m*-K_4Ga, (b) *C*2/*m*-K_4Ga, (c) $P2_1/c$-K_3Ga, (d) $P2_1/m$-K_3Ga, (e) $P2_1/m$-K_2Ga, (f) *P*-3*m*1-K_2Ga.

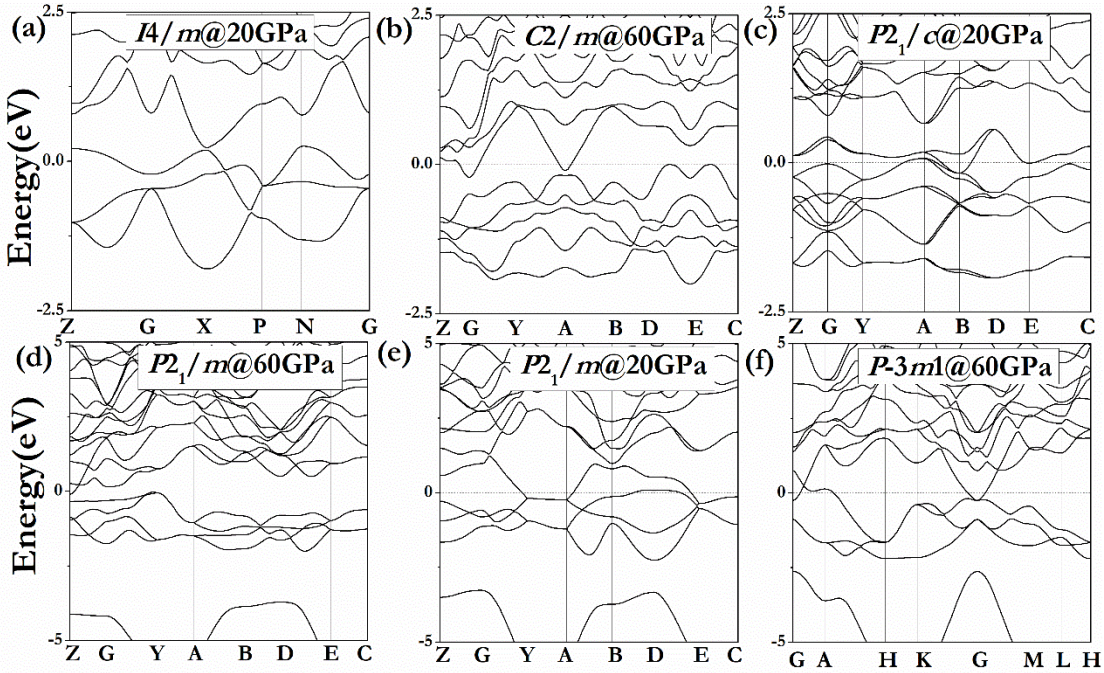

Figure S6: Calculated band structures of Ga-rich compounds: (a) *P*2/*m*-KGa_2, (b) *C*2/*c*-KGa_2, (c) *I*4/*mmm*-KGa_4, (d) *Pnma*-KGa_4.

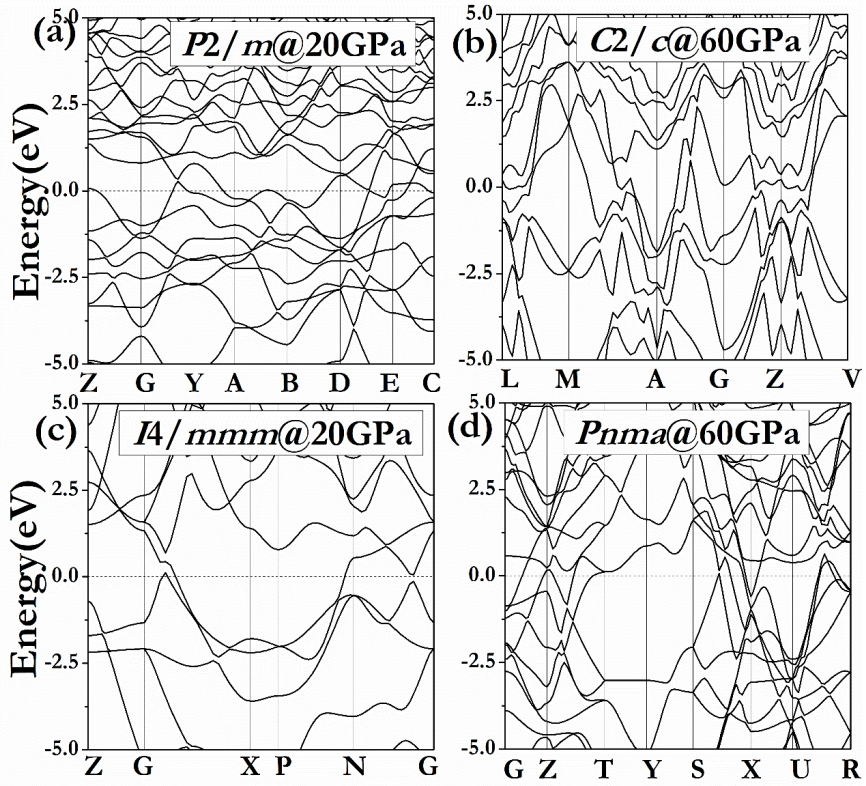

Figure S7: Calculated band structures of *F*d-3*m*-KGa.

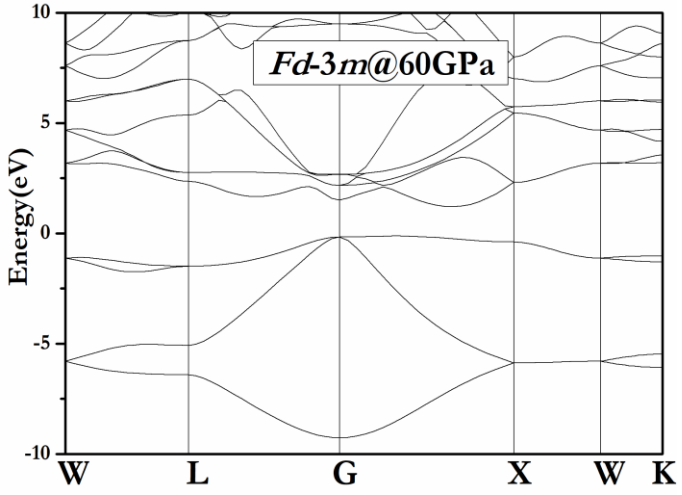

Figure S8: Electron localization function (ELF) of (a) *I*4/*m*-K_4Ga, *P*-3*m*1-K_2Ga and *C*2/*c*-KGa_2.

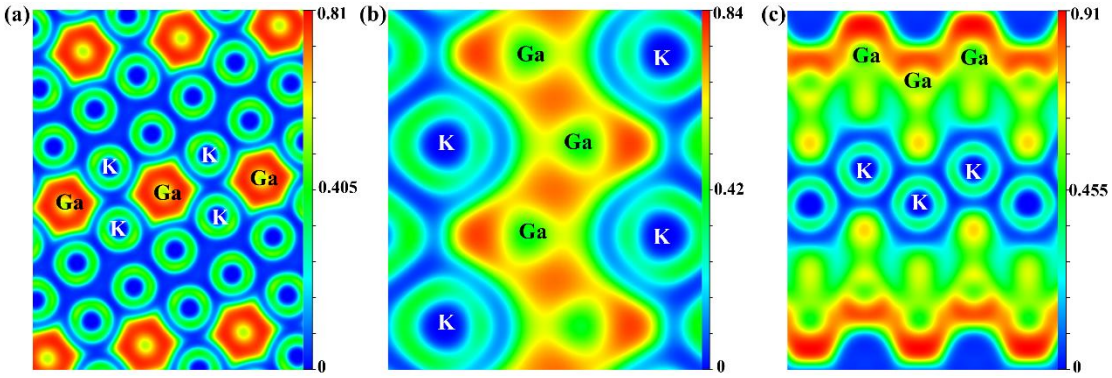

Figure S9: Electron localization function (ELF) of (a) *P*2_1/*c*-K_3Ga, (b) *P*2_1/*m*-K_3Ga and (c) *Fd*-3*m*-KGa.

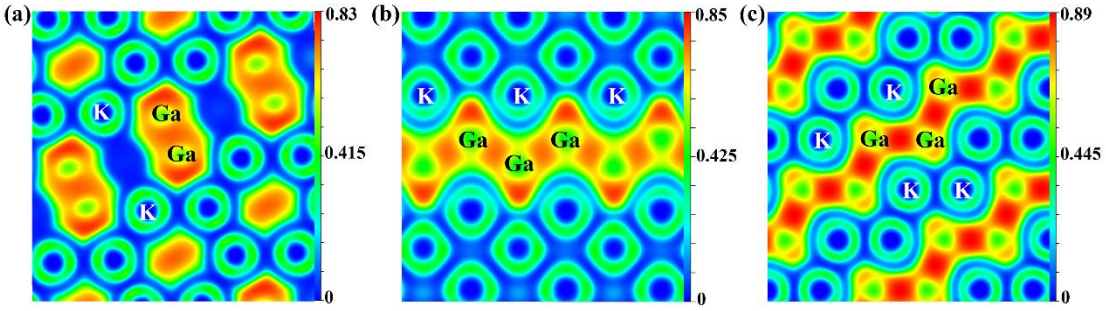

Table S1 Structural parameters of K−Ga system at selected pressures.

Space group pressure	Lattice parameters (Å, °)	Atomic coordinates (fractional)	Sites
K_4Ga (*I*4/*m*)	a=b=6.79730	K1 0.41477 0.79496 2.00000	8h
20 GPa	α=β=γ=90	Ga1 0.00000 1.00000 1.00000	2a
K_4Ga (*C*2/*m*)	a=9.44790	K1 0.30343 -1.00000 0.58496	4i
	b=4.92500	K2 0.18812 -1.50000 0.12889	4i
	c=9.10120	K3 0.00000 -1.24759 0.50000	4h
60 GPa	α=γ=90	K9 0.68093 -2.00000 0.85062	4i
	β=133.5045	Ga1 0.44695 -1.50000 0.82018	4i
K_3Ga ($P2_1/c$)	a=5.57750	K1 0.77864 0.25137 0.25267	4e
	b=7.89120	K2 0.27052 0.49840 0.01945	4e
20 GPa	c=9.87150	K3 -0.13494 0.62798 -0.62484	4e
	α=γ=90	Ga1 0.59607 0.89056 0.10810	4e
K_3Ga ($P2_1/m$)	a=5.56840	K1 0.72871 -0.25000 -0.16915	2e
	b=4.04190	K3 0.22588 -0.25000 -0.11132	2e
	c=5.55680	K7 0.93540 -0.25000 0.34819	2e
60 GPa	α=γ=90	Ga1 1.55663 -0.75000 -0.39782	2e
	β=75.8530		
K_2Ga ($P2_1/m$)	a=5.64490	K1 0.00039 0.25000 -0.30071	2e
	b=4.52120	K5 0.68817 0.25000 0.03549	2e
	c=5.32180	Ga1 0.38946 -0.75000 -0.59164	2e
20 GPa	α=γ= 90		
	β=113.2820		
K_2Ga (*P*-3*m*1)	a= b=3.98870	K1 2.00000 1.00000 -1.25672	2c
	c=5.55120	K2 1.33333 0.66667 -1.41099	2d
100 GPa	α=β=90	Ga1 1.66667 1.33333 -1.06214	2d
	γ=120		
KGa (*Fd*-3*m*)	a=b=c=5.84330	K1 -0.50000 0.50000 1.00000	8a
100 GPa	α=β=γ=90	Ga1 0.00000 0.00000 1.50000	8b
KGa_2 (*P*2/*m*)	a=7.24590	K1 1.00000 1.00000 0.00000	1a
	b=5.48560	K2 0.41054 1.00000 0.20420	2m
	c=5.58290	K3 0.50000 0.50000 0.50000	1h
20 GPa	α=γ=90	Ga1 0.82679 0.77979 0.40204	4o
	β=103.5388	Ga2 0.31444 0.50000 -0.05413	2n
		Ga5 1.09071 0.50000 0.23007	2n
KGa_2 (*C*2/*c*)	a=2.51830	K1 2.50000 0.20451 1.25000	4e
	b=15.08250	Ga1 2.00000 0.38684 1.25000	4e
	c=5.07080	Ga2 2.00000 0.03435 1.25000	4e
60 GPa	α=γ =90		
	β=121.1710		
KGa_4 (*I*4/*mmm*)	a= b=4.00100	K1 2.00000 0.00000 -1.00000	2a
	c=10.69830	Ga1 1.00000 0.00000 -0.38953	4e
20 GPa	α=β=γ= 90	Ga9 0.50000 0.00000 -0.75000	4d
KGa_4 (*Pmma*)	a=4.28670	K1 0.25000 0.50000 -1.12868	2f
	b=5.33500	Ga1 0.25000 0.71158 -0.61093	4k
60 GPa	c=5.90950	Ga5 0.75000 1.00000 -0.09203	2e
	α=β=γ=90	Ga9 0.25000 1.00000 -0.30676	2e

Table S2 Bader analysis for K−Ga system at selected pressures.

Structure	Atom	Number	Charge value(e)	δ(e)
K_4Ga (*I*4/*m*) 20GPa	Ga	1	4.8237	-1.8237
	K1	4	6.544075	+0.455925
K_4Ga (*C*2/*m*) 60GPa	Ga	2	4.46525	-1.46525
	K1	2	6.6403	+0.3597
	K2	2	6.6013	+0.3987
	K3	2	6.6686	+0.3314
	K4	2	6.6245	+0.3755
K_3Ga ($P2_1/c$) 20GPa	Ga	4	4.4502	-1.4502
	K1	4	6.5085	+0.4915
	K2	4	6.5430	+0.457
	K3	4	6.4983	+0.5017
K_3Ga ($P2_1/m$) 60GPa	Ga	2	4.04005	-1.04005
	K1	2	6.6414	+0.3586
	K2	2	6.6727	+0.3273
	K3	2	6.6459	+0.3541
K_2Ga ($P2_1/m$) 20GPa	Ga	2	4.05585	-1.05585
	K1	2	6.4789	+0.5211
	K2	2	6.4652	+0.5348
K_2Ga (*P*-3*m*1) 100GPa	Ga	2	3.74885	-0.74885
	K1	2	6.63615	+0.36385
	K2	2	6.6150	+0.385
KGa (*Fd*-3*m*) 100GPa	Ga	2	3.4521	-0.4521
	K	2	6.5479	+0.4521
KGa_2 (*P*2/*m*) 20GPa	Ga1	2	3.3315	-0.3315
	Ga2	2	3.3105	-0.3105
	Ga3	2	3.20155	-0.20155
	Ga4	2	3.3361	-0.3361
	K1	1	6.4064	+0.5936
	K2	2	6.3880	+0.612
	K3	1	6.5483	+0.4517
KGa_2 (*C*2/*c*) 60GPa	Ga1	2	3.3617	-0.3617
	Ga2	2	3.0718	-0.0718
	K1	2	6.5665	+0.4335
KGa_4 (*I*4/*mmm*) 20GPa	Ga1	2	3.21405	-0.21405
	Ga2	2	3.08715	-0.08715
	K1	1	6.3975	+0.6025
KGa_4 (*Pmma*) 60GPa	Ga1	2	3.1370	-0.1370
	Ga2	2	3.1592	-0.1592
	Ga3	2	3.2238	-0.2238
	Ga4	2	2.9950	+0.005
	K1	2	6.4850	+0.515