



Bulk modulus of molecular crystals

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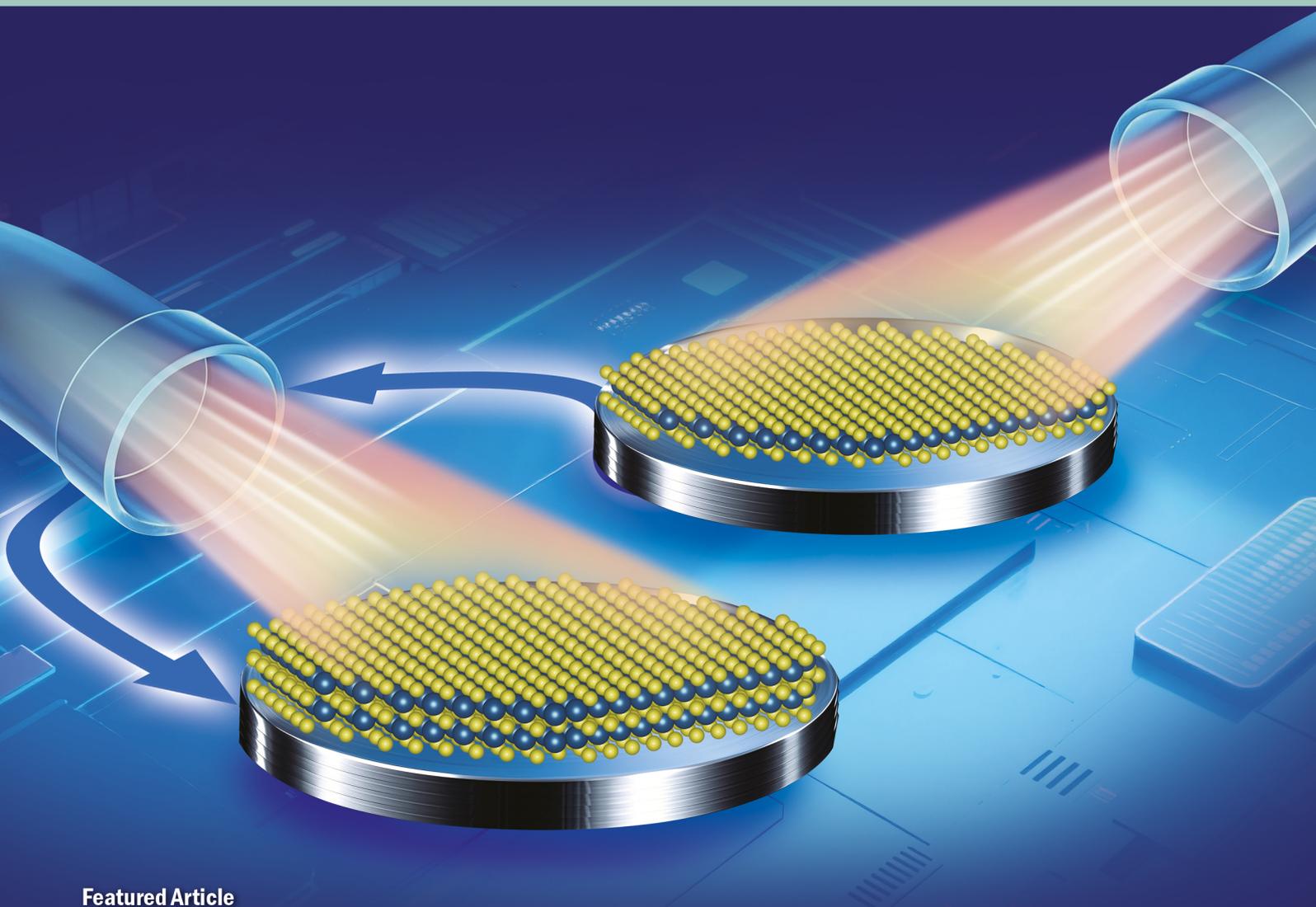
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Bulk modulus of molecular crystals

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Bulk modulus is a constant that measures the incompressibility of materials, which can be obtained in high pressure experiment by fitting the equations of state (EOS), like third-order Birch–Murnaghan EOS (BM EOS) and Vinet EOS. Bulk modulus reflects the intermolecular interaction inside molecular crystals, making it useful for researchers to design novel high pressure materials. This review systematically examines bulk moduli of various molecular crystals, including rare-gas solids, di-atom and triplet-atom molecules, saturated organic molecules, and aromatic organic crystals. Comparisons with ionic crystals are presented, along with an analysis of connections between bulk modulus and crystal structures.

Keywords: high pressure, bulk modulus, molecular crystal, intermolecular interaction

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1. Introduction

1.1. Molecular crystals at high pressure

Molecular crystals are primarily composed of small molecules interconnected through intermolecular interactions such as van der Waals interactions, which exhibit lower binding strength compared with covalent or ionic interactions. These weak intermolecular interactions result in enhanced compressibility under pressure. Such high compressibility gives rise to a greater variety of distinct high-pressure structures and generates more materials with new properties under high pressure.^[1] High pressure enables to reduce the intermolecular distances,^[2,3] increase the density of electron,^[4,5] or change the energetic ordering of the outer atomic orbitals of molecules.^[6,7] In term of the different compressibility of molecular crystals, applying pressure could produce interesting phenomena, like pressure-induced polymerization,^[8–10] pressure-driven phase transition,^[11–13] and even molecule dissociations.^[14,15]

In recent decades, high-pressure responses of molecular crystals have been widely investigated across chemistry, physics, biology, geoscience, and materials science. For instances, the water-ice system has been found to have a very rich phase diagram with about twenty stable and metastable phases, which is of crucial importance for understanding the entire diversity of nature.^[16] Unsaturated molecular crystals like nitrogen,^[17–19] carbon monoxide,^[20,21] nitriles,^[22] alkene,^[23–25] alkyne,^[26–28] and aromatic compounds^[29–33] tend to polymerize under high pressure, providing a new method to develop novel materials.

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1.2. Bulk modulus and the equations of state

Bulk modulus (B) quantifies the degree of deformation,^[34–36] and can be used to probe the phase transition^[37–39] and reaction^[40] of molecular crystals in high pressure experiment, making it significant to characterize the physical property of a material system.^[41–45] The bulk modulus is defined as

$$B = -\frac{dP}{dV/V} = -\frac{dP}{d \ln V}, \quad (1)$$

where P is pressure, and V is volume. A reduced bulk modulus in materials directly correlates with enhanced compressibility, demonstrating weakened intermolecular bonding forces between constituent atoms/molecules.^[46]

High pressure bulk modulus is normally obtained by fitting the equations of state (EOS), the formula that describes the equilibrium state by a series of thermodynamic variables like pressure, volume, and temperature.

If we assume that bulk modulus is a linear function of pressure as

$$B = B_0 + B'_0 P, \quad (2)$$

$$B'_0 = \partial B / \partial P, \quad (3)$$

where B_0 is the bulk modulus at $P = 0$ GPa and B'_0 is the first derivative of the bulk modulus. Then we can derive the Murnaghan EOS (MU) by integrating formula (1) and substituting it into the boundary condition of $P = 0$ GPa.^[44,47] It can be represented as

$$P = \frac{B_0}{B'_0} \left[\left(\frac{V}{V_0} \right)^{-B'_0} - 1 \right], \quad (4)$$

where B_0 is the bulk modulus at $P = 0$ GPa, B'_0 is the first derivative of the bulk modulus, and V_0 is the cell volume at $P = 0$ GPa. Murnaghan EOS is widely used for calculating metamorphic phase equilibria because it provides a simple algebraic resolution of P in terms of V , but it is considered only suitable for low pressure^[48] (4 GPa suggested by Kumar)^[49] or compressions up to about 10% ($V/V_0 > 0.9$).^[41] The most popular EOS is the Birch–Murnaghan EOS (BM EOS).^[50,51] BM EOS is based on Murnaghan’s theory of finite deformations to describe the effect of hydrostatic pressure upon the elastic coefficients of an isotropic body.^[50] It defines the Eulerian finite strain of uniformly compressed cubic as

$$f = -\varepsilon_E = \frac{1}{2} \left[\left(\frac{V}{V_0} \right)^{-\frac{2}{3}} - 1 \right]. \quad (5)$$

Then substitute formula (5) into the third-order expansion of Helmholtz free energy by Eulerian finite strain^[44]

$$\Delta F \cong af^2 + bf^3, \quad (6)$$

where F is the Helmholtz free energy, a and b are two elastic constants. Combining with the definition of B and B' , the third-order Birch–Murnaghan EOS that contains both bulk modulus and its first derivative is represented as

$$P = \frac{3}{2} B_0 \left[\left(\frac{V}{V_0} \right)^{-\frac{2}{3}} - \left(\frac{V}{V_0} \right)^{-\frac{5}{3}} \right] \times \left\{ 1 + \frac{3}{4} (B'_0 - 4) \left[\left(\frac{V}{V_0} \right)^{-\frac{2}{3}} - 1 \right] \right\}, \quad (7)$$

where B_0 is the bulk modulus at $P = 0$ GPa, B'_0 is the first derivative of the bulk modulus, and V_0 is the cell volume at $P = 0$ GPa. BM EOS was developed for isotropic materials and was commonly applied to all solids, especially metals. Fitting accuracy may decrease under non-hydrostatic pressure conditions or deviations from isotropic compression criteria.

Another conventional EOS is Vinet EOS, which is also called the “universal” EOS.^[52–54] Vinet EOS is based on a semi-universal relationship for interatomic potentials, assuming wave-function-overlap interactions dominate during compression for all solids. This approach simplifies treatment of diverse bonding types, enabling formulation of a unified EOS framework.^[52]

The Vinet EOS can be derived from the relation^[55] between energy and the interatomic separation distance as

$$E(r) = E(r)_0 \left(1 + \frac{r-r_0}{l} \right) \times \exp \left(-\frac{r-r_0}{l} \right), \quad (8)$$

where $E(r)$ is the total energy, r is the interatomic separation distance, and l is a scaling length. Considering the relation of P and $E(r)$, we will get

$$P = -\frac{\partial E(r)}{\partial V} = \frac{E(r)_0}{3l^2} V^{-\frac{2}{3}} \left(-V^{-\frac{1}{3}} + V_0^{\frac{1}{3}} \right)$$

$$\times \exp \left(\frac{-V^{-\frac{1}{3}} + V_0^{\frac{1}{3}}}{l} \right). \quad (9)$$

Combining formula (9) with formulas (1) and (3), the Vinet EOS can be represented as

$$P = 3B_0 \left(\frac{V}{V_0} \right)^{-\frac{2}{3}} \left[1 - \left(\frac{V}{V_0} \right)^{\frac{1}{3}} \right] \times \exp \left\{ \frac{3}{2} (B'_0 - 1) \left[1 - \left(\frac{V}{V_0} \right)^{\frac{1}{3}} \right] \right\}, \quad (10)$$

where B_0 is the bulk modulus at $P = 0$ GPa, B'_0 is the first derivative of the bulk modulus, and V_0 is the cell volume at $P = 0$ GPa. Vinet EOS has a better performance in organic crystals, but has a larger error when considering the influence of temperature.^[54] Besides, Vinet EOS requires modifications for strong compression to remain “universal” for different systems.^[56]

As shown in Table 1, Holzapfel summarized other common equations of states,^[48] like the EOS form of the generalized strain expansion (GS2),^[48] the linearization form EOS that represents the Hugoniot curves related to linear u_s-u_p relations (MS2),^[57] the EOS based on an effective Lennard–Jones potential used by Grüneisen (MG3),^[58] the EOS based on a generalized Born–Mayer type effective potential (GBM),^[48] the EOS based on the effective Morse potential (Emo),^[48] the Vinet EOS modified by replacing the Born type exponential repulsion with an effective Thomas–Fermi type potential (HO2),^[59] the EOS that can perfectly match with the free electron Fermi-gas limit ($B'_\infty = 5/3$) which can’t be approached for other EOS under high pressure (H12).^[59]

Table 1. Commonly used equations of states forms with their parameter relations. B_0 is the bulk modulus at $P = 0$ GPa, B'_0 is the first derivative of the bulk modulus, V_0 is the cell volume at $P = 0$ GPa, and $x = (V/V_0)^{1/3}$.

Name	Equations of states	B'_0
MU ^[47]	$P = \frac{3}{c} B_0 \cdot x^{-c} \cdot (1-x^c)$	$\frac{c}{3}$
BM ^[50]	$P = \frac{3}{2} B_0 \cdot x^{-7} \cdot (1-x^2) \cdot (1+c(x^{-2}-1))$	$4 + \frac{4}{3}c$
GS2 ^[48]	$P = \frac{3}{n} B_0 \cdot x^{-2n-3} \cdot (1-x^n) \cdot (1+c(x^{-n}-1))$	$n + 2 + \frac{2n}{3}c$
MS2 ^[57]	$P = B_0(1-x^3) \cdot (1+c(1-x^3))$	$4c - 1$
MG3 ^[58]	$P = \frac{3}{n} B_0 \cdot x^{-n} \cdot (1-x^n)$	$\frac{2m-n}{3}$
GBM ^[48]	$P = \frac{3B_0}{c-n-1} \cdot x^{-2} \cdot (1-x^{-n-1}) \cdot e^{-c(1-x)} \cdot e^{c(1-x)}$	$\frac{4}{3} + \frac{c^2-c-(n+1)^2}{3(c-n-1)}$
Emo ^[48]	$P = \frac{6}{c} B_0 \cdot x^{-2} \cdot (1-e^{-c(2)(1-x)}) \cdot e^{c(1-x)}$	$1 + \frac{1}{2}c$
Vinet ^[52]	$P = 3B_0 \cdot x^{-2} \cdot (1-x) \cdot e^{c(1-x)}$	$1 + \frac{2}{3}c$
HO2 ^[59]	$P = 3B_0 \cdot x^{-5} \cdot (1-x) \cdot e^{c(1-x)}$	$3 + \frac{2}{3}c$
H12 ^[59]	$P = 3B_0 \cdot x^{-5} \cdot (1-x) \cdot e^{cx(1-x)} \cdot e^{c_0(1-x)}$	$3 + \frac{2}{3}(c+c_0)$

Researchers need to understand the applicable pressure range and assumptions of the EOSs to avoid over-fitting. Both Murnaghan EOS, BM EOS and Vinet EOS are semi-empirical equations, because their assumptions like isotropic compression or energy relation have not been strictly expanded to other fields, although they have shown good fitting ability for different systems. As comparisons, Vinet EOS normally has a

better result for strong compression due to its strong exponential term, which represents the ability for materials to store energy by deformation under strong compression. Third-order BM EOS also has a good fitting result for strong compression, while Murnaghan EOS was considered not suitable for compression of process greater than 4 GPa because its low exponent term.^[49]

However, there are also some cases in which Murnaghan EOS has the best fitting result, or these three EOSs have similar results. For example, Pravica *et al.* found that Murnaghan EOS had the lowest relative error for the compression of cyclohexane up to 40 GPa,^[60] though the Murnaghan EOS was suggested to be accurate up to 4 GPa.^[49] Vlasic *et al.* found that there is almost no difference for Vinet EOS, BM EOS and a four-parameter EOS^[61] when considering the structure II gas

hydrate system.^[62]

1.3. High pressure device

The EOS is normally measured by shock-wave and static high-pressure experiments with crystallographic techniques. There are two types of conventional static high-pressure devices, Paris–Edinburgh cell (PE cell)^[63,64] and diamond anvil cell (DAC)^[65] for *in situ* neutron and synchrotron or lab x-ray diffraction measurements, respectively. DAC is the most popular device that can produce a super high pressure up to 1 TPa.^[66] Paris–Edinburgh cell is suitable for mg-scale experiments, which can reach pressure up to 40 GPa.^[67–69] Researchers can obtain the cell parameters at different pressures and then obtain the bulk modulus by fitting the equations of state.^[70]

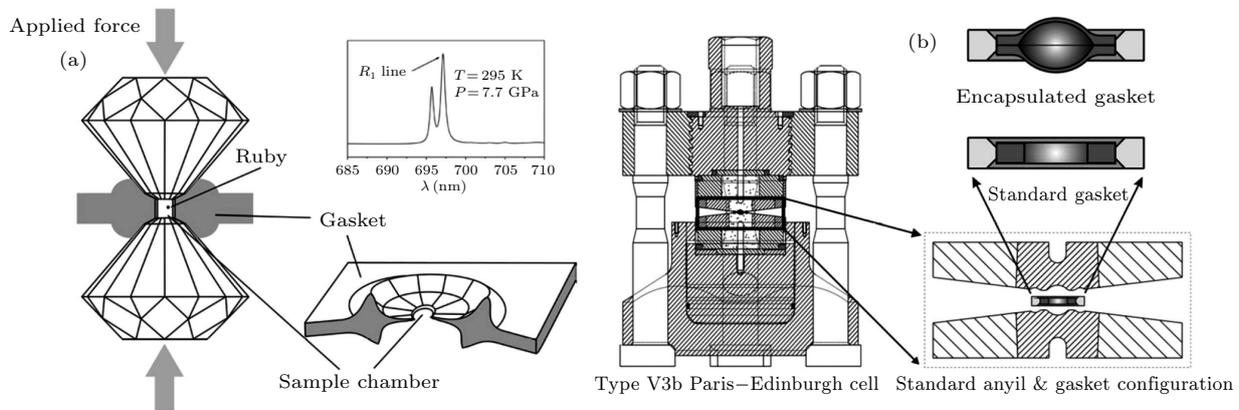


Fig. 1. The structure of (a) diamond anvil cell^[71] and (b) Paris–Edinburgh cell.^[71]

2. Bulk modulus of different molecular crystals

2.1. Rare-gas solids

The bulk modulus of monoatomic molecules is important for the investigation of giant planet, and also for high pressure experiment, because rare gases are commonly used as pressure transmitting media (PTM) in DAC.^[72] Generally, the high-pressure structure of rare gases is hexagonal close packed (hcp), which is different from the cubic close packed (fcc) low pressure phase. It is interesting that neon remains a fcc phase up to 208 GPa without evidence of the formation of hcp phase,^[73] indicating weaker three-body-exchange interactions which cause phase transitions of other rare gases.^[74]

The bulk moduli of rare gases are assorting in Table 2. Helium has the smallest bulk modulus of 0.65 GPa for fcc phase and 3 GPa for hcp phase.^[75] Neon has a larger bulk modulus, with the reported data from 1.07 GPa,^[73] 0.74 GPa,^[76,77] to 12 GPa^[75] for fcc phase. Argon's bulk modulus ranges from 2.4 GPa^[76,78] to 6 GPa^[75] for fcc phase, and has a bulk modulus of 13 GPa for hcp phase,^[75] and a value of 3 GPa was reported for the mixed phase of fcc and hcp.^[79] Krypton has bulk modulus of 1.6 GPa^[80]

or 3.3 GPa^[79] for mixed phase even under a pressure of 140 GPa,^[80] and has a bulk modulus of 5.5 GPa for fcc phase and 23 GPa for hcp phase.^[75] Xenon has the largest bulk modulus in rare-gas solids of 3.6 GPa,^[81] 4.5 GPa^[82] or 7 GPa^[75] for fcc phase, while having the bulk modulus of 4.3 GPa^[81] or 22 GPa^[75] for hcp phase and 4.3 GPa^[79] for the mixed phase.

Considering the similar crystal structures for rare gases, we can generally find that atomic radius has the major influence on bulk modulus. The larger atom radius leads to a stronger dispersion interaction,^[83] which will induce a larger bulk modulus. Besides, the hcp phase usually has a larger bulk modulus than the fcc phase, indicating a more compact packing structure under high pressure. The deduction about the relationship between bulk modulus and atomic radius can be extended to more complex molecular crystals. The difference between the reported data reflects the error of the experimental data and the fitting processes. Due to the deviation of experiment and EOS, it is difficult to determine the accuracy of bulk modulus only by the fitting results. DFT calculation^[84] and acoustic techniques such as Brillouin scattering or ultrasonic interferometry^[85,86] may be needed for auxiliary judgment.

Table 2. Bulk modulus of rare-gas solids.

Name	Structure	Pressure range (GPa)	EOS & Model	B_0 (GPa)	B'_0
Helium ^[75]	fcc	1–10	BM	0.65	2
Helium ^[75]	hcp	1–80	BM	3	12
Neon ^[76,77]	fcc	4.7–14.4	Murnaghan	0.74	7.1
Neon ^[73]	fcc	1–208	Vinet	1.07	8.4
Neon ^[75]	fcc	1–110	Murnaghan	12	4.2
Argon ^[76,78]	fcc	1.2–8.2	Murnaghan	2.4	7
Argon ^[79]	fcc+hcp	1–128	Mie–Grüneisen	3	7.2
Argon ^[75]	fcc	1–20	BM	6	4
Argon ^[75]	hcp	20–114	BM	13	3.5
Krypton ^[80]	fcc+hcp	1–140	BM	1.6	7.1
Krypton ^[79]	fcc+hcp	1–128	Mie–Grüneisen	3.3	7.2
Krypton ^[75]	fcc	1–20	Murnaghan	5.5	3.8
Krypton ^[75]	hcp	20–140	Murnaghan	23	3.5
Xenon ^[81]	fcc	3.7–70	BM	3.6	5.5
Xenon ^[81]	hcp	70–127	BM	4.3	4.9
Xenon ^[79]	fcc+hcp	1–128	Mie–Grüneisen	4.3	6.5
Xenon ^[82]	fcc	1–60	BM	4.5	5.6
Xenon ^[75]	fcc	1–20	Vinet	7	5.8
Xenon ^[75]	hcp	20–175	Vinet	22	3

2.2. Di-atom and triplet-atom molecules

The bulk modulus of diatoms molecules (H_2 and N_2) listed in Table 3 are both small but the latter (2.69 GPa)^[87] is larger than the former (0.162 GPa),^[88] which agrees with the above result that the bulk modulus is dependent on the molecular size. Ice under high pressure exhibits a larger bulk modulus (12–260 GPa),^[89–93] which arises from the hydrogen-bonding interactions within the crystalline lattice. For comparison, the low pressure phase carbon dioxide has a bulk modulus of 2.93 GPa^[94] or 6 GPa,^[95] representing the enhancement ef-

fect of hydrogen bond on bulk modulus. The unusual high bulk modulus (87 GPa, 131 GPa, and 365 GPa)^[95] of high pressure phase carbon dioxide was explained by the transformation from molecular crystal to covalent crystal,^[95–97] the different fitting pressure range,^[98] or the inaccuracy of the experiment caused by the hysteresis of phase transition.^[99] The enhancement effect of hydrogen bond was also observed in complex systems. For example, Dreger *et al.*^[100] found that 5,5'-bistetrazole-1,1'-diolate has a negative linear compressibility of the a axis caused by the strong hydrogen bonding interaction along the a axis.

Table 3. Bulk modulus of di-atom and triplet-atom molecules.

Name	Pressure range (GPa)	EOS & Model	B_0 (GPa)	B'_0
Hydrogen ^[88]	10–109	Vinet	0.162	6.813
Hydrogen ^[88] (Cal)	120–350	Mie–Grüneisen	0.999	5.799
δ phase nitrogen ^[87]	5.7–43.9	Olinger & Halleck ^[89]	2.69	3.93
ϵ phase nitrogen ^[87]	5.7–43.9	Olinger & Halleck ^[89]	2.98	3.78
Ice VII ^[89]	3.0–8.0	Olinger & Halleck ^[89]	12.54	5.56
Ice VII ^[90]	0–13	Vinet	27.8	2.8
Ice VII ^[90]	13–66	Vinet	97	3
Ice VII ^[90]	66–106	Vinet	260	7.3
Ice VII ^[91]	2–13.7	BM	13.8	5.9
Ice VII ^[91]	2–13.7	Vinet	13.6	6.2
Ice VII ^[91]	2–13.7	H12	13.7	6.0
mixed phase ice ^[92]	2.2–170	Vinet	4.26	7.75
Ice VIII ^[93] (300 K)	2.2–18	BM	20.4	4.7
Ice VIII ^[91] (93 K)	2–13.7	BM	18.7	5.7
Ice VIII ^[91] (93 K)	2–13.7	Vinet	18.5	6.0
Ice VIII ^[91] (93 K)	2–13.7	H12	18.6	5.9
Ice VIII ^[91] (196 K)	2–13.7	BM	15.6	6.2
Ice VIII ^[91] (196 K)	2–13.7	Vinet	15.4	6.4
Ice VIII ^[91] (196 K)	2–13.7	H12	15.6	6.2
Mixed phase CO ₂ ^[94]	1–51.4	BM	2.93	7.8
Phase I CO ₂ ^[95]	1–11	BM	6	6.1
Phase III CO ₂ ^[95]	11–50	BM	87	3.3
Phase II CO ₂ ^[95] (> 500 K)	20–50	BM	131	2.1
Phase V CO ₂ ^[95] (> 1600 K)	40–50	BM	365	0.8

2.3. Saturated organic molecules

The bulk moduli of saturated organic molecules are listed in Table 4. Generally, we can find that the larger molecules have a larger bulk modulus. For example, ethane (25.9 GPa or 71.1 GPa),^[101] heptane (14.5 GPa),^[102] cyclohexane (12 GPa)^[60] and cubane (14.5 GPa)^[103] have a larger bulk modulus than methane. However, the data of ethane is a little surprising. Normally, the bulk modulus of small molecular crystals with van der Waals interactions only is smaller than 15 GPa and the bulk modulus of ionic crystals is larger than 20 GPa.

Besides, what we need to note is that researchers propend to fix the B'_0 at 4 when having too limited data to fit the EOS. This means ignoring the influence of B'_0 ,^[104] $B'_0 \approx 4$ is actually a common value for ionic crystals and metals, but fixing it at 4 will likely result in a larger B_0 , especially for molecular crystals.^[48,105] For example, Lin *et al.*^[106] found that the fitted B_0 of ammonia borane will increase from 4.8 GPa to 9.8 GPa if

the fixed B'_0 decreases from 10 to 6.4, and Fan *et al.*^[107] found that the calcium-lead fluorapatite solid solution will have a B_0 smaller by about 10–20 GPa if not fixed the B'_0 at 4. As shown in Table 3, Hazen *et al.*^[108] and Sun *et al.*^[109] fixed B'_0 at 4 for methane and obtained a series of bulk moduli for different phases, such as 4.9 GPa for fcc phase,^[108] or 7.9 GPa for rhombohedral phase,^[110] 23.7 GPa^[109] or 23.1 GPa for simple cubic phase,^[111] and 28.5 GPa for a high-pressure phase,^[109] which will mathematically make B_0 larger. In comparison, when B'_0 is not fixed, the bulk modulus of $C(CN)_4$ ^[112] and $C[Si(CH_3)_3]_4$ ^[113] is 4.4 and 5.4, respectively. It is reasonable to infer that the bulk modulus of methane should be smaller than $C(CN)_4$ and $C[Si(CH_3)_3]_4$ without B'_0 fixed. Therefore, in consideration of the increasing size of substituent group, we probably could find a positive relation between the bulk modulus and molecular volume, in consistent with the previous conclusion.

Table 4. Bulk modulus of saturated organic molecules.

Name	Pressure range (GPa)	EOS & Model	B_0 (GPa)	B'_0
$C(CN)_4$ ^[112]	0.1–14.7	BM	4.4	18
[121]Tetramantane ^[114]	1–13	BM	5.4	18.75
$C[Si(CH_3)_3]_4$ ^[113]	1–5	BM	5.5	15
Fcc CH_4 ^[108]	1.6–5.2	Murnaghan	4.9	4 (fixed)
Rhombohedral CH_4 ^[109]	11–27	BM	7.8	4 (fixed)
Rhombohedral CH_4 ^[110]	7–13	BM	7.9	4 (fixed)
Simple cubic CH_4 ^[109]	19–69	BM	23.7	4 (fixed)
Simple cubic CH_4 ^[111]	17–85	BM	23.1	4 (fixed)
High-pressure phase CH_4 ^[109]	94–202	BM	28.5	4 (fixed)
C_2H_6 ^[101]	2.7–13.4	BM	25.9	9.2
C_2H_6 ^[101]	13.4–110	BM	71.1	3.5
Heptane ^[102]	1.7–10	BM	14.5	4 (fixed)
NH_3BH_3 ^[106]	1.6–5	BM	8	6.4 (Cal)
1,1-diamino-2,2-dinitroethene ^[115]	1–4.5	BM	10.1	14.3
ϵ -CL-20 ^[116]	1–12	BM	11.5	11.2
Cubane ^[103]	1–60	BM	14.5	6.2
α -glycine ^[117]	0.2–6.4	Vinet	19.5	6.5
<i>l</i> -cystine ^[118]	0–6.4	BM	29.1	4 (fixed)
Cyclohexane ^[60]	1–40	BM	12	14.5
Cyclohexane ^[60]	1–40	Vinet	9.9	8.1
Cyclohexane ^[60]	1–40	Murnaghan	22.9	4.8

2.4. Aromatic organic molecules

Aromatic organic molecules are always hot spots in the research on high-pressure chemistry. The pressure-induced polymerization of aromatic compounds enables the production of novel extended carbon materials, for example, the one-dimension diamondoid nanothreads with high strength and stiffness.^[119] In the studies of aromatics under high pressure, scientists found that the structures of polymerized samples are highly related to the high-pressure molecular structures before reaction. Therefore, the comprehensive studies of the crystalline structures and phase transitions under high pressure are greatly helpful for understanding the interactions between aro-

matic molecules.^[120] The details of aromatic organic crystals are assorting in Table 5, arranging in an ascending order of bulk modulus.

Generally, aromatic molecular crystals have a small bulk modulus, normally ranging from 2 GPa to 10 GPa, as shown in Table 5. Benzene as the typical model of aromatics was proven to have two high pressure phases, the phase I with *Pbca* space group^[121] and the phase II with *P2₁/c* space group^[122] in a herringbone packing structure. It has a bulk modulus of 7.8 GPa for phase I^[123] and 13.9 GPa for phase II at room temperature.^[123] Aniline (5.4 GPa)^[124] and deuterated phenol (5.8 GPa)^[125] have a similar bulk modulus and packing structure to benzene due to the similar size.

With the increasing size of the conjugated coplanar structure, the bulk modulus correspondingly increased. For example, the bulk modulus of naphthalene,^[126] anthracene,^[127,128] tetracene^[128] and pentacene^[128] is 7.9 GPa, 8.4–8.8 GPa, 9 GPa and 9.6 GPa, respectively. There is a similar situation for phenylenes, biphenyl (4.3 GPa),^[105] *para*-terphenyl (7.2 GPa),^[105] *para*-quaterphenyl (8.3 GPa),^[105] *para*-quinquephenyl (9.3 GPa)^[105] and *para*-sexiphenyl (10 GPa),^[105] with the increasing number of benzene rings. In addition, comparing the two types of aromatic molecules, the biphenyl structure linked by the rotatable σ bond has a relatively smaller bulk modulus, which means the biphenyl compounds are more easily compressed under high pressure.

The size of molecules also makes a contribution to the bulk modulus of other aromatic crystals. The *s*-

triazine (6.3 GPa)^[139] and pyridine (6.2 GPa or 6.4 GPa)^[140] have a similar bulk modulus compared with benzene because of the similar molecules, while 1,3,5-triethynylbenzene (10 GPa)^[137] has a larger bulk modulus and a larger volume. Besides, the strong hydrogen bonds in the crystal structure of 3,3'-diamino-4,4'-azoxyfurazan (9.1 GPa),^[141] melamine (12 GPa),^[142] 1H-tetrazole (13.6 GPa),^[144] 2,5-furandicarboxylic acid (21 GPa),^[145] and 1,5-diamino-1H-tetrazole (23 GPa),^[146] make them have a larger bulk modulus than similar volume molecules, such as bibenzyl (4.9 GPa),^[131] benzene (7.8 GPa),^[123,132] and naphthalene (7.9 GPa).^[126] Azulene has a much larger bulk modulus of 18.1 GPa^[138] than its tautomer naphthalene, which can be explained by its differential charge distribution and large dipole moment (1.08 D).^[148]

Table 5. Bulk modulus of aromatic organic crystals.

Name	Pressure range (GPa)	EOS & Model	B_0 (GPa)	B'_0
$C_2H_2 \cdot C_6H_6$ ^[129]	1–20	BM	2	17
<i>para</i> -xylene ^[130]	0.1–4.7	BM	3.5	14
Biphenyl ^[105]	1–6	Murnaghan	4.3	8.4
Bibenzyl ^[131]	1–20	Vinet	4.9	9.3
Aniline ^[124]	1.6–7.3	Vinet	5.4	9.9
Phase I benzene ^[123]	0.9–2.2	BM	7.8	4.7
Phase II benzene ^[132] (540 K)	1–26	Vinet	5.5	8.5
Phase II benzene ^[123]	2.5–24.1	BM	13.9	4
Full deuterated phenol ^[125]	1–20	Vinet	5.8	8.6
Azobenzene ^[133]	1–9.5	Vinet	5.8	9.5
Fluorene ^[134]	1–14	Murnaghan	6.2	7.9
Naphthalene-Octafluoronaphthalene ^[135]	1–20.6	Vinet	7.1	9.2
Anthracene-Octafluoronaphthalene ^[135]	1–25.5	Vinet	7.2	8.6
1,3,5-triamino-2,4,6-trinitrobenzene ^[136]	1–10	Vinet	7.2	13.9
<i>para</i> -terphenyl ^[105]	1–6	Murnaghan	7.2	6.1
Naphthalene ^[126]	1–5.6	Vinet	7.9	7.5
<i>para</i> -quaterphenyl ^[105]	1–6	Murnaghan	8.3	6.4
Anthracene ^[128]	1–9	Murnaghan	8.4	6.3
Anthracene ^[127]	1–22.6	Murnaghan	8.8	6.0
Tetracene ^[128]	1–9	Murnaghan	9	7.9
<i>para</i> -quinquephenyl ^[105]	1–6	Murnaghan	9.3	7.5
Pentacene ^[128]	1–9	Murnaghan	9.6	6.4
<i>para</i> -sexiphenyl ^[105]	1–6	Murnaghan	10	5.6
1,3,5-triethynylbenzene ^[137]	0.1–3.6	BM	10	5
Azulene ^[138]	2.7–7.7	BM	18.1	3.9
<i>s</i> -triazine ^[139]	1–7	Vinet	6.3	10.8
Phase II pyridine ^[140]	0.9–2.5	BM	6.4	8.7
Phase III pyridine ^[140]	1.2–2.7	BM	6.2	8.1
Thiophene ^[31]	0–20	BM	8.1	6.7
3,3'-diamino-4,4'-azoxyfurazan ^[141]	2–12.1	BM	9.1	8.3
Perdeuterated melamine ^[142]	0–5	BM	12.0	7.8
2,6-diethynylpyridine ^[143]	0.7–5.4	BM	13	4 (fixed)
1H-tetrazole ^[144]	0.1–2	BM	13.6	4 (fixed)
2,5-furandicarboxylic acid ^[145]	0.2–10.8	BM	21	4 (fixed)
1,5-diamino-1H-tetrazole ^[146]	1–40	BM	23	4 (fixed)
1,4-difluorobenzene ^[147]	4.3–9.4	BM	27	4 (fixed)

Additionally, we inferred that the π - π stacking interaction of aromatic crystals may make a different influence on bulk modulus. As shown in Table 5, we can find that the bulk modulus of aromatic molecules is smaller than the

non-aromatic molecules with similar size, representing that aromaticity makes a smaller bulk modulus. This could be attributed to the weakened repulsion induced by π -orbital interaction.^[149–151] Besides, the softening of the repulsive

wall in aromatic species makes the extra stabilization and lower bulk modulus for aromatic molecular crystals.^[149,152] It is worth noting that *para*-xylene has a smaller bulk modulus of 3.5 GPa, which may be attributed to the C–H··· π interaction between methyl and adjacent benzene ring, in addition to π – π stacking interaction of benzene rings.^[130,153,154] The different bulk modulus of cocrystals can also illustrate the influence of molecule size and π stacking interaction. For example, naphthalene-octafluoronaphthalene (7.1 GPa)^[135] and anthracene-octafluoronaphthalene (7.2 GPa)^[135] have the similar bulk modulus with naphthalene but C₂H₂·C₆H₆ have a small bulk modulus (2 GPa)^[129] than benzene. This is because that octafluoronaphthalene has a similar size with naphthalene, anthracene has a larger size and π stacking interaction that almost cancel the influence of each other, and acetylene has a small size than benzene that makes a small bulk modulus.

2.5. Typical ionic crystals

For comparison, we also list some bulk moduli of ionic crystals. Ionic crystals normally consist of Coulomb interaction, which has an inverse-square relationship between the interaction strength and interaction distance. The different degree of strength attenuation with interaction distance between Coulomb interaction and van der Waals interactions^[52] makes the different correlation between crystal structure and bulk modulus. For example, the bulk moduli of alkali halides represent a negative correlation with the atomic radius as shown in Table 6,^[155] while rare-gases solids represent a positive correlation. We can also find that most of the ionic crystals have a large B_0 with a B'_0 between 4 and 6, indicating a dense structure and low compressibility of ionic crystals.

Table 6. Bulk modulus of typical ionic crystals.

Name	Pressure range (GPa)	EOS & Model	B_0 (GPa)	B'_0
LiI ^[155]	0–40	H11 ^[156]	17.3	5.56
LiBr ^[155]	0–40	H11	23.5	5.23
LiCl ^[155]	0–40	H11	29.7	4.59
LiF ^[155]	0–40	H11	66.5	4.30
NaI ^[155]	0–40	H11	14.9	5.58
NaBr ^[155]	0–40	H11	19.5	5.29
NaCl ^[155]	0–40	H11	23.7	4.81
NaF ^[155]	0–40	H11	46.5	4.64
KI ^[155]	0–40	H11	11.5	5.58
KBr ^[155]	0–40	H11	14.6	5.33
KCl ^[155]	0–40	H11	17.4	4.93
KF ^[155]	0–40	H11	30.2	4.82
RbI ^[155]	0–40	H11	10.5	5.76
RbBr ^[155]	0–40	H11	13.2	5.57
RbCl ^[155]	0–40	H11	15.6	5.29
RbF ^[155]	0–40	H11	26.7	5.27
CsI ^[155]	0–40	H11	11.9	5.93
CsBr ^[155]	0–40	H11	14.3	5.80
CsCl ^[155]	0–40	H11	16.7	5.58
Phase B1 KBr ^[157]	0–2.3	Vinet	14.2	5.5 (fixed)
Phase B2 KBr ^[157]	0–227	Vinet	13.8	5.65
Phase B1 KCl ^[157]	0–2.6	Vinet	17.1	5.5 (fixed)
Phase B2 KCl ^[157]	0–233	Vinet	17.4	5.63
NH ₄ I ^[158]	1.3–68	BM	18.8	4.22
Sb ₂ S ₃ ^[159]	0–10	BM	26.9	7.9
Sb ₂ S ₃ ^[160]	0–5	BM	27.2	6 (fixed)
Sb ₂ S ₃ ^[160]	0–5	BM	65	4 (fixed)
Sb ₂ Se ₃ ^[161]	0–51	BM	30	6.1
Bi ₂ S ₃ ^[162]	0–10	BM	36.6	6.4
Bi ₂ S ₃ ^[163]	0–50	BM	38.9	5.5
β -Ba(OH) ₂ ^[164]	0–8.1	BM	35	12
MgO ^[165]	0.8–52.2	BM	160.2	3.99
CeO ₂ ^[166]	0–40	Birch	230	4.0
CaIrO ₃ -type Al ₂ O ₃ ^[167]	120–180	BM	249	4 (fixed)

3. Conclusion

Generally, molecular crystals exhibit lower bulk moduli compared to ionic crystals. Rare-gas solids have the simi-

lar bulk modulus and compressibility with organic crystals, which should be taken into consideration in the high-pressure experiment of organics when using the rare-gas as pressure

transition medium. Analysis of molecular crystals reveals a correlation between bulk modulus and molecular size, with hydrogen bonding interactions showing measurable influence on bulk modulus. Although dipole moment and stacking interactions also contribute to bulk modulus, these factors appear secondary to molecular size and hydrogen bond in most molecular crystal systems. This review aims to provide foundational insights for establishing the relationship between bulk modulus and crystal structures. The quantitative relation between the bulk modulus and the size of molecules as well as the molecular interactions needs to be investigated in the future.

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JUST FOR AUTHORS
— CHINESE PHYSICS B

Chinese Physics B

Volume 34 Number 6 June 2025

Contents

TOPICAL REVIEW — Structures and properties of materials under high pressure

066201 Bulk modulus of molecular crystals

Xudong Jiang, Yajie Wang, Kuo Li and Haiyan Zheng

068301 Iron nitrides: High-pressure synthesis, nitrogen disordering and local magnetic moment

Yu Tao and Li Lei

SPECIAL TOPIC — Structures and properties of materials under high pressure

066102 Layer-dependent structural stability and electronic properties of CrPS₄ under high pressure

Jian Zhu, Dengman Feng, Liangyu Wang, Liang Li, Fangfei Li, Qiang Zhou and Yalan Yan

066105 Morphology-tuned phase transition of MnO₂ nanorods under high pressure

Xue-Ting Zhang, Chen-Yi Li, Hui Tian, Xin-Yue Wang, Zong-Lun Li and Quan-Jun Li

066202 High-pressure synthesis of an oxynitride perovskite CeNbO₂N with Nb⁴⁺ charge state

Shengjie Liu, Xubin Ye, Zhao Pan, Jie Zhang, Shuai Tang, Guangkai Zhang, Maocai Pi, Zhiwei Hu, Chien-Te Chen, Ting-Shan Chan, Cheng Dong, Tian Cui, Yanping Huang, Zhenhua Chi, Yao Shen and Youwen Long

066203 Measurement of the eutectic point of Fe–C alloy under 5 GPa

Ting Zhang, Xiuyan Wei, Zuguang Hu, Jianyun Yang, Duanwei He, Khalid Nabulsi and Guodong (David) Zhan

066204 Structural regulation and optical behavior of zero-dimensional Cu(I)-based organometallic halides under pressure

Runnan Ye, Jingtian Wang, Jiayi Yang, Xuchen Wang, Junce Lei, Wenya Zhao, Yufan Meng, Guanjun Xiao and Bo Zou

066205 Band gap engineering and vibrational properties of van der Waals semiconductor ZnPSe₃ under compression

Rouqiong Su, Yuying Li, Chunhua Chen, Yifang Yuan and Haizhong Guo

067403 Pressure-induced superconductivity in Bi-doped BaFe₂(As_{1-x}Bi_x)₂ single crystals

Chang Su, Wuhao Chen, Wenjing Cheng, Jiabin Si, Qunfei Zheng, Jinlong Zhu, Lingyi Xing and Ying Liu

(Continued on the Bookbinding Inside Back Cover)

SPECIAL TOPIC — Artificial intelligence and smart materials innovation: From fundamentals to applications

066101 General-purpose moment tensor potential for Ga–In liquid alloys towards large-scale molecular dynamics with *ab initio* accuracy

Kai-Jie Zhao and Zhi-Gong Song

067101 Unveiling the thermal transport mechanisms in novel carbon-based graphene-like materials using machine-learning potential

Yao-Yuan Zhang, Meng-Qiu Long, Sai-Jie Cheng and Wu-Xing Zhou

068101 Surface-pitted TiN nanoparticles for direct absorption solar collectors

Heng Zhang, Yuchun Cao, Xiaowen Chen, Qihang Yang, Ning Chen and Xiaohu Wu

068102 Performance analysis of porous solar absorbers with high-temperature radiation cooling function

Haiyan Yu, Anqi Chen, Mingdong Li, Ahali Hailati, Xiaohu Wu and Xiaohan Ren

068903 Interfacial design and thermoelectric properties of C₃N₄-C₂₀ molecular junctions based on quantum interference

Shutao Hu, Meng Qian, Gang Zhang and Bei Zhang

SPECIAL TOPIC — Ultrafast physics in atomic, molecular and optical systems

063201 Relativistic terahertz laser pulse from photon deceleration in a plasma wakefield

Jie Cai, Minjian Wu, Yixing Geng, Huangang Lu, Han Wen, Liqi Han, Yanying Zhao, Jinqing Yu and Xueqing Yan

063202 High-order harmonic generation of methane in an elliptically polarized field

Shu-Shan Zhou, Yu-Long Li, Zhi-Xue Zhao, Man Xing, Nan Xu, Hao Wang, Jun Wang, Xi Zhao and Mu-Hong Hu

063301 Experimental manipulation of fine structures in high harmonic spectrum of aligned CO₂ molecules

Ge-Wen Wang, Yi-Wen Zhao, Yi-Chen Wang, Jing Ma, Bo-Dun Liu, Wei Jiang, Hong-Jing Liang and Ri Ma

063302 Tuning the laser-dressed attosecond transient absorption spectra of a singly excited helium state using a shaped attosecond pulse with a spectral minimum

Yong Fu, Feier Xu and Cheng Jin

063702 A Rb–Cs dual-species magneto-optical trap

Shiyao Shao, Qing Li, Lihua Zhang, Bang Liu, Zhengyuan Zhang, Qifeng Wang, Jun Zhang, Yu Ma, Tianyu Han, Hanchao Chen, Jiadou Nan, Yiming Yin, Dongyang Zhu, Yajun Wang, Dongsheng Ding and Baosen Shi

SPECIAL TOPIC — Advanced magnonics

- 067104 A two-stage injection locking amplifier based on a cavity magnonic oscillator**
Mun Kim, Chunlei Zhang, Chenyang Lu, Jacob Burgess and Can-Ming Hu
- 067506 First- and second-order magnonic topologies in the ferromagnetic breathing SSH model modulated by non-Hermitian effects**
Huasu Fu, Lichuan Zhang, Rami Mrad, Yuee Xie and Yuanping Chen
- 067507 Magnon behavior in YIG film under microwave excitation investigated by Brillouin light scattering**
Guofu Xu, Kang An, Wenjun Ma, Xiling Li, C. K. Ong, Chi Zhang and Guozhi Chai
- 067508 Bifurcation of the bound states in the continuum in a dissipative cavity magnonic system**
Xinlin Mi, Lijun Yan, Bimu Yao, Shishen Yan, Jinwei Rao and Lihui Bai
- 068502 Control of the magnonic excitation under the joint mechanism of magnetostrictive effect and magnetocrystalline anisotropy**
Saisai Yu, Junbo Liu and Hao Xiong

INSTRUMENTATION AND MEASUREMENT

- 066106 A large-area scintillation neutron detector based on WLSF and SiPM readout**
Xiao-Hu Wang, Yang-Tu Lu, Bin Tang, Xiu-Ku Wang, Shao-Jia Chen, Ze-Ren Li and Zhi-Jia Sun

REVIEW

- 067702 Positive and negative electrocaloric effects**
Hongrui Xu and Jiping Huang

RAPID COMMUNICATION

- 067505 Multiferroicity and thermal expansion of the layered metal–organic framework $[\text{NH}_4\text{Cl}]_2[\text{Ni}(\text{HCOO})_2(\text{NH}_3)_2]$**
Dan Cheng, Yingjie He, Shuang Liu, Na Su and Young Sun
- 068103 Two-step growth of 4-inch multilayer MoS_2 wafers**
Yang-Kun Zhang, Yu-Chen Wang, Wei Yang, Dong-Xia Shi, Luo-Jun Du and Guang-Yu Zhang
- 068701 Simple robot swarm with magnetic coupling connections can collaboratively accomplish collective tasks**
Xingyu Ma, Chuyun Wang, Jing Wang, Huaicheng Chen, Gao Wang and Liyu Liu

GENERAL

- 060201 Coherent states associated with integral multi-index Mittag–Leffler functions**
Dušan Popov

060202 An ADP-based robust control scheme for nonaffine nonlinear systems with uncertainties and input constraints

Shijie Luo, Kun Zhang and Wenchao Xue

060203 Global dynamics and optimal control of SEIQR epidemic model on heterogeneous complex networks

Xiongdin Liu, Xiaodan Zhao, Xiaojing Zhong and Wu Wei

060301 Ground state of SU(3) spin-orbit coupled soft-core Bose gas

Jia Liu, Jing Feng, Ya-Jun Wang, Xiao-Fei Zhang and Xue-Ying Yang

060302 Surface solitons in Kerr-type nonlinear media with chirped lattices

Xiaoyang Wang, Huilian Wei, Xuefei Zhang and Tianfu Xu

060303 Witnessing the distribution of sources in quantum networks via hierarchical nonlocality

Shu-Yuan Yang, Jin-Chuan Hou and Kan He

060501 Synchronous dynamics of robotic arms driven by Chua circuits

Guoping Sun, Mingxin Xu, Guoqiang Jin and Xufeng Wang

060701 Testing algorithm for the computation of the transverse emittance of the ion beams generated by the ECR mVINIS ion source based on a pepper-pot method

Viktor Jocić, Igor Telečki and Ivan Trajić

ATOMIC AND MOLECULAR PHYSICS

063701 Sub-Doppler cooling of magnesium fluoride molecules

Jin Wei, Di Wu, Taojing Dong, Chenyu Zu, Yong Xia and Jianping Yin

ELECTROMAGNETISM, OPTICS, ACOUSTICS, HEAT TRANSFER, CLASSICAL MECHANICS, AND FLUID DYNAMICS

064201 Correlated Rydberg electromagnetically induced transparencys

Lei Huang, Peng-Fei Wang, Han-Xiao Zhang, Yu Zhu, Hong Yang and Dong Yan

064202 High-efficiency Yb³⁺-doped fiber laser with highly optical nonlinear Bi₄Br₄-based saturable absorber

Mengyuan Liu, Yechao Han, Qi Liu, Hao Teng, Xiwei Huang, Xiaowei Xing, Xiangyu Qiao, Guojing Hu, Xiao Lin, Haitao Yang, Zhiyi Wei and Wenjun Liu

064203 Multi-wavelength and transversely mode-switchable fiber laser based on ring-core fiber Bragg grating

Ya-Jun Jiang, Yu-Hui Su, Jia-Xin Gao, Feng Zhou, Li-Qin Cheng, Kang-Wei Pan, Bin-Chuan Sun, Li Shen, De-Xing Yang and Jian-Lin Zhao

064204 Polarization-sensitive nonlinear optical diffraction

Jianluo Chen, Lihong Hong, Yu Zou, Jiacheng Li and Zhi-Yuan Li

064401 Thermal investigation of water-based radiative magnetized micropolar hybrid nanofluid flow subject to impacts of the Cattaneo–Christov flux model on a variable porous stretching sheet with a machine learning approach

Showkat Ahmad Lone, Zehba Raizah, Rawan Bossly, Fuad S. Alduais, Afrah Al-Bossly and Arshad Khan

064601 Fractional order nonlinear dynamics modeling of air spring

Zheming Kang, Shaofang Wen, Jing Chen, Yongjun Shen and Yunfei Liu

064701 Study on adaptive mesh method in the problem of underwater shock waves near water surface

Fang Wang, Xinpeng Yuan and Jianzhu An

064702 Adsorption-modulated dynamical stability of nanobubbles at the solid–liquid interface

Guiyuan Huang, Lili Lan, Binghai Wen, Li Yang and Yong Yang

PHYSICS OF GASES, PLASMAS, AND ELECTRIC DISCHARGES

065101 Development characteristics of dielectric barrier discharge channels with rotating high-voltage electrodes

Hui Jiang, Jinyu Tang and Yufei Han

065201 General relaxation model for a homogeneous plasma with spherically symmetric velocity space

Yanpeng Wang, Shichao Wu and Peifeng Fan

CONDENSED MATTER: STRUCTURAL, MECHANICAL, AND THERMAL PROPERTIES

066103 Deciphering the capacity degradation mechanism in lithium manganese oxide batteries

Lin Wang, Shijie Li, Na Li and Wei-Li Song

066104 Improved temperature localization by hollowing plasmonic nanofocusing cones

Jiaming Zhang and Jinglai Duan

066301 Anomalous lattice vibration in monolayer MoS₂ induced by DUV laser: A first-principles investigation

Weidong Wang, Renhui Liu, Ye Zhang, Huaihong Guo, Jianqi Huang, Zhantong Liu, Heting Zhao, Kai Wang, Bo Zhao and Teng Yang

066302 Laser power-induced Fermi-level shift in graphene/Al₂O₃ under ambient atmosphere: Toward neutralizing unintentional graphene doping

Jamal Q. M. Almarashi, Mohamed K. Zayed, Hesham Fares, Heba Sukar, Takao Ono, Yasushi Kanai and Mohamed Almokhtar

CONDENSED MATTER: ELECTRONIC STRUCTURE, ELECTRICAL, MAGNETIC, AND OPTICAL PROPERTIES

- 067102 Interacting Dirac semi-metal state in nonsymmorphic Kondo-lattice compound CeAgSb₂**
Da-Liang Guo and Huan Li
- 067103 Quantum oscillations and nontrivial topology in unfilled skutterudite IrSb₃**
Yang Yang, Xinyao Li, Feihong Guan, Majeed Ur Rehman, Wei Ning, Xiangde Zhu and Mingliang Tian
- 067201 Prolonging carrier lifetime in P-type 4H-SiC epilayer by thermal oxidation and hydrogen annealing**
Ruijun Zhang, Mingkun Zhang, Guoliang Zhang, Yujian Chen, Jia Liu, Ziqian Tian, Ye Yu, Peng Zhao, Jiafa Cai, Xiaping Chen, Dingqu Lin, Shaoxiong Wu, Yuning Zhang, Xingliang Xu, Rongdun Hong and Feng Zhang
- 067202 Planar Hall effect without chiral anomaly in layered topological semimetal candidate GaGeTe**
Cheng Wang, Ankang Zhu, Ziyi Fan, Peng Huang, Xue Liu, Xuegang Chen, Yuyan Han, Zheng Chen, Xiangde Zhu, Mingliang Tian and Wenshuai Gao
- 067301 Random flux manipulating topological phase transitions in Chern insulators**
Jinkun Wang and Wu-Ming Liu
- 067302 In-plane optical anisotropy of InGaN/GaN quantum disks in nanowires investigated by reflectance difference spectroscopy**
Tingting Wei, Jinling Yu, Zhu Diao, Zhaonan Li, Shuying Cheng, Yunfeng Lai, Yonghai Chen and Chao Zhao
- 067303 Modulating electronic properties of carbon nanotube via constructing one-dimensional vdW heterostructures**
Wenqi Lv, Weili Li, Wei Ji and Yanning Zhang
- 067304 Low leakage current β -Ga₂O₃ MOS capacitors with ALD deposited Al₂O₃ gate dielectric using ozone as precursor**
Zheng-Yi Liao, Pai-Wen Fang, Xing Lu, Gang Wang and Yan-Li Pei
- 067401 Strongly tunable Ising superconductivity in van der Waals NbSe_{2-x}Te_x nanosheets**
Jingyuan Qu, Guojing Hu, Cuili Xiang, Hui Guo, Senhao Lv, Yechao Han, Guoyu Xian, Qi Qi, Zhen Zhao, Ke Zhu, Xiao Lin, Lihong Bao, Yongjin Zou, Lixian Sun, Haitao Yang and Hong-Jun Gao
- 067402 Dimensional crossover from quasi-2D to 3D superconductivity in (Li,Fe)OHFeSe_{1-x}S_x driven by chemical pressure**
Yuxin Ma, Munan Hao, Qi Li, Ke Ma, Haodong Li, Duo Zhang, Ruijin Sun, Shifeng Jin and Changchun Zhao

067501 Orbital magnetic field effect on spin waves in a triangular lattice tetrahedral antiferromagnetic insulator

Pi-Ye Zhou, Xiao-Hui Li and Yuan Wan

067502 Crystal structure, magnetic properties, and tunable Kondo effect in a new compound $\text{Nd}_5\text{ScSb}_{12}$

Yi-Ran Li, Na Li, Ping Su, Hui Liang, Kai-Yuan Hu, Ying Zhou, Dan-Dan Wu, Yan Sun, Qiu-Ju Li, Xia Zhao, Xue-Feng Sun and Yi-Yan Wang

067503 Complex magnetic and transport properties of EuBi_2 single crystal

Ping Su, Hui Liang, Yi-Ran Li, Huan Wang, Na Li, Kai-Yuan Hu, Ying Zhou, Dan-Dan Wu, Yan Sun, Qiu-Ju Li, Jin-Jin Hong, Xia Zhao, Xue-Feng Sun and Yi-Yan Wang

067504 A design for an antiferromagnetic material based on self-assembly for information storage

Si-Yan Gao, Yi-Feng Zheng, Shu-Qiang He, Haiping Fang and Yue-Yu Zhang

067701 Molecular dynamics simulations of ferroelectricity in P(VDF-TrFE)

Mengyuan Tang, Chuhan Tang, Sheng-Yi Xie and Fuxiang Li

INTERDISCIPLINARY PHYSICS AND RELATED AREAS OF SCIENCE AND TECHNOLOGY

068201 Al-Zr dual-doping enhancing the electrochemical performance of spinel LiMn_2O_4 cathodes

Wei Wu, Yuhui Cui, Yuxin Zheng, Fei Huang, Hong Li and Liang Yin

068401 Simulation of the non-Hermitian Kitaev chain by electrical circuits

Jiali Xu, Hao Geng, Abdul Wahab, Xiaosen Yang, Yuee Xie and Yuanping Chen

068402 Marked improvement of photoelectric response performance based on CNTF/AgNSF/PZT pyroelectric photodetector: A comprehensive study

Bocheng Lv, Xiyu Hong, Jinqun Wei, Mohsin Rafique and Zhe Li

068501 A high-sensitivity deep-junction single-photon detector for near-infrared imaging

Yuanhao Bi, Dajing Bian, Ming Li and Yue Xu

068702 Depolymerization mechanism of microtubule revealed by nucleotide-dependent changes of longitudinal and lateral interactions

Bingbing Zhang, Ziling Huo, Jiaxi Li, Jingyu Qin and Yizhao Geng

068703 Adaptive regulation effectively mitigates the spread of rumors

Fu-Zhong Nian, Zhen Wang and Yi Jia

068704 Effects of information and policy regulation on green behavior propagation in multilayer networks: Modeling, analysis, and optimal allocation

Xian-Li Sun and Ling-Hua Zhang

068901 Understanding subway passenger alighting and boarding dynamics: Experiments and modelling

Chenrui Xuan, Yuxin Li, Yu Wang, Eric Wai Ming Lee, Yi Ma and Wei Xie

068902 Influence of negative information dissemination and vaccination behavioral decision-making on epidemic spreading in a three-layer network

Liang'an Huo and Leyao Yin

068904 Zero-determinant game design for preventing double-spending in IOTA

Yin-Feng Chen and Zhong-Hua Fu

GEOPHYSICS, ASTRONOMY, AND ASTROPHYSICS

069701 JCMT observations of CO, SO₂, and a U-line in circumstellar envelopes of four O-rich AGB stars

Yanan Feng, Xiaohu Li, Sheng-Li Qin, Tom J. Millar, Ryszard Szczerba, Zhenzhen Miao and Juan Tuo

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