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This agreement ("Agreement") is a legal agreement between the user ("you" or "User") and the limo software development team ("Development Team") concerning the use of the limo software ("Software"). Please read all the terms and conditions of this Agreement carefully before installing or using this Software. If you do not agree to any terms of this Agreement, do not install or use this Software.

1 Software License

- 1.1 The Development Team grants you a non-exclusive, non-transferable, limited license to install and use the Software on computers you own or control, subject to the terms and conditions of this Agreement.
- 1.2 The Software is available for academic use and commercial use. You should select the appropriate use type based on your actual needs.

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- 2.1 Academic use refers to using the Software for academic research, teaching, or non-commercial personal research.
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Stress-strain curve: LEI M, SUN G, YANG G, WEN B. A computational mechanical constitutive modeling method based on thermally-activated microstructural evolution and strengthening mechanisms[J]. International Journal of Plasticity, 2024, 173

doi:https://doi.org/10.1016/j.ijplas.2024.103881

FLAPW single-point energy calculation and structure optimization: ZHANG S, GAO X, SONG H, WEN B. An adaptive preconditioning scheme for the self-consistent field iteration and generalized stacking fault energy calculations[J]. Computer Physics Communications, 2024, 304

doi:https://doi.org/10.1016/j.cpc.2024.109300

High-temperature elastic constants: WEN B, SHAO T, MELNIK R, et al. Temperature and pressure dependent geometry optimization and elastic constant calculations for arbitrary symmetry crystals: Applications to MgSiO3 perovskites[J]. Journal of Applied Physics, 2013, 113(10)

doi: https://doi.org/10.1063/1.4794360

SHAO T, WEN B, MELNIK R, et al. Temperature dependent elastic constants for crystals with arbitrary symmetry: Combined first principles and continuum elasticity theory[J]. Journal of Applied Physics, 2012, 111(8)

doi: https://doi.org/10.1063/1.4704698

SHAO T, WEN B, MELNIK R, et al. Temperature dependent elastic constants and ultimate strength of graphene and graphyne[J]. J Chem Phys, 2012, 137(19): 194901.

doi: https://doi.org/10.1063/1.4766203

mechanical property: WEN B, XU B, WANG Y, et al. Continuous strengthening in nanotwinned diamond[J]. npj Computational Materials, 2019, 5(1)

doi: https://doi.org/10.1038/s41524-019-0256-2

FENG X, XIAO J, WEN B, et al. Temperature-dependent hardness of zinc-blende structured covalent materials[J]. Science China Materials, 2021, 64(9): 2280-2288.

doi:https://doi.org/10.1007/s40843-020-1620-4

SUN G, FENG X, WU X, et al. Is hardness constant in covalent materials?[J]. Journal of Materials Science & Technology, 2022, 114: 215-221.

doi:https://doi.org/10.1016/j.jmst.2021.10.032

XIAO J, YANG H, WU X, et al. Dislocation behaviors in nanotwinned diamond[J]. Sci Adv, 2018, 4(9): eaat8195.

doi:https://doi.org/ 10.1126/sciadv.aat8195

FENG X, SUN G, ZHANG S, WEN B. A unified non-empirical strength model[J]. Frontiers in Materials, 2023, 9

doi:https://doi.org/10.3389/fmats.2022.1049956

2.3 Users under academic use can freely use the standard functionality modules of the Software, but the Development Team reserves the right to charge fees for advanced features or modules.

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- 3.1 Commercial use refers to using the Software for any commercial purposes, including but not limited to product development, commercial research, providing analysis services to third parties, or other profit-oriented activities.
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- 3.3 You may not use the Software for commercial purposes or commercialize the calculated data generated by the Software without the written consent of the Development Team.

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- 4.2 You may not reverse engineer, decompile, decode, or attempt to extract the source code of the Software in any way, nor modify, adapt, adapt, or create derivative works based on the Software.

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- 5.1 You may not sell, rent, transfer, or redistribute copies of the Software in any way.
- 5.2 You may not share or publicly display the Software on any public or commercial network.
 - 5.3 You may not use the Software for any illegal or unauthorized activities.

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- 6.1 The Software may collect and use certain data, including but not limited to technical information and usage data, to help improve products and services. All data collection and use will comply with the Development Team's privacy policy.
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7.1 Any data, results, or outputs generated using the Software (hereinafter referred to

as "User-Generated Data") are your property.

- 7.2 You agree to take full responsibility for the accuracy, completeness, and legality of your User-Generated Data. The Development Team is not responsible for any direct or indirect consequences arising from the use of User-Generated Data.
- 7.3 The Development Team reserves the right to collect and use anonymous User-Generated Data to improve the Software and other related services. Such data collection will not include any information that can identify the user.
- 7.4 You agree not to use User-Generated Data obtained using the Software for any illegal activities or in violation of this Agreement.

8. Software Updates and Support

- 8.1 The Development Team reserves the right to update, modify, or terminate any part of the Software at any time without notice.
- 8.2 The Software is provided "as-is" and "as available," with no warranty of bug fixes, functionality enhancements, or user support.

9 Disclaimer

- 9.1 The Software is provided "as-is" without any express or implied warranties, including but not limited to warranties of merchantability, fitness for a particular purpose, and non-infringement.
- 9.2 The Development Team does not warrant that the Software's functions will meet your requirements or expectations, nor that the Software's operation will be uninterrupted or error-free.

10 Limitation of Liability

10.1 In no event shall the Development Team be liable for any special, incidental, indirect, or consequential damages (including but not limited to loss of profits, business interruption, loss of information, etc.) arising out of the use or inability to use the Software or User-Generated Data, even if the Development Team has been advised of the possibility of such damages.

10.2 In any event, the Development Team's total liability to you under this Agreement shall not exceed the amount you paid for the Software (if any).

11 Termination

- 11.1 This Agreement will automatically terminate if you violate any terms of this Agreement without any notice.
- 11.2 Upon termination of the Agreement, you must cease using the Software and destroy all copies of the Software.

12 Governing Law

12.1 This Agreement shall be governed by and construed under the laws of the People's Republic of China, without regard to its conflict of law principles.

13 Entire Agreement

13.1 This Agreement constitutes the entire agreement between you and the Development Team regarding using the Software and supersedes all prior oral or written understandings or agreements.

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13.2 If any provision of this Agreement is deemed invalid or unenforceable, that

provision shall be modified to the minimum extent necessary to make it valid and

enforceable under applicable law, and the remaining provisions of the Agreement shall

remain in full force and effect.

Acceptance of Agreement

By clicking the "Accept" or "Agree" button, installing, or using the Software, you

confirm that you have read, understood, and agree to be bound by this Agreement.

Name:

Research Group and Group Leader:

University/Research Institution:

Email:

Date(yyyy-mm-dd):