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Prediction of Structurally Stable Two-Dimensional $AuClO_2$ with High Thermoelectric Performance

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Supplementary Information

Mechanical Properties. The mechanical properties of $AuClO_2$ monolayer has been performed in VASPKIT code using the strain-stress method.[1] As shown in Table S1, four independent elastic constants C_{ij} are deduced for the orthorhombic lattice with a $P222_1$ space group, which satisfy the mechanical stability criteria $C_{11} > 0$, $C_{33} > 0$, and $C_{11} \times C_{22} > C_{12}^2$. The low elastic constants are relevant to the low lattice thermal conductivity.[2] It can be evidently defined from Fig. S7 that $AuClO_2$ possesses strong mechanical anisotropy for the huge variety of Bulk modulus (B), Young's modulus (E), and Shear modulus (G) along different directions.

Calculation Method. The lattice thermal conductivity κ_L has been calculated with a 14 × 14 × 1 *q*-point mesh in ShengBTE code. The required harmonic and anharmonic interatomic force constants (IFCs) are both computed by VASP combined with PHONOPY and THIRDORDER.PY script with a 3 × 2 × 1 supercell.[3] The IFC2 is obtained through the finite-difference approach in PHONOPY, and the IFC3 is carried out in THIRDORDER.PY script with the same approach. The interactions up to third-nearest neighbors are considered for anharmonic IFCs.

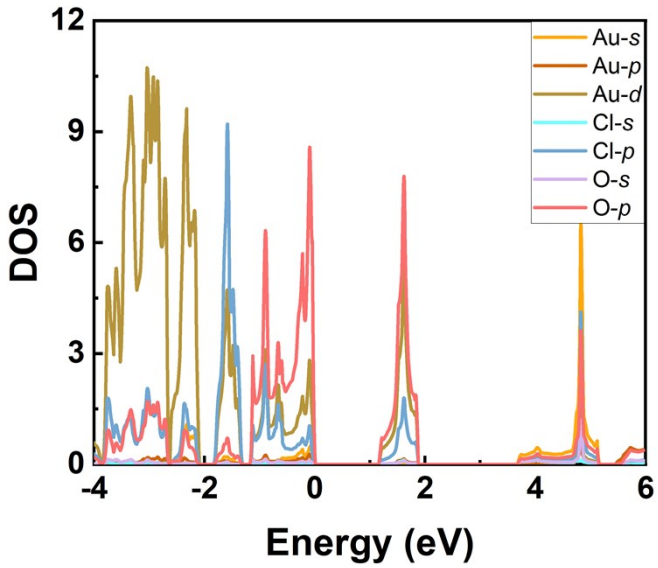

Figure S1. The calculated partial electronic density of states (PDOS) projected to valence orbitals under GGA-PBE exchange-correction function.

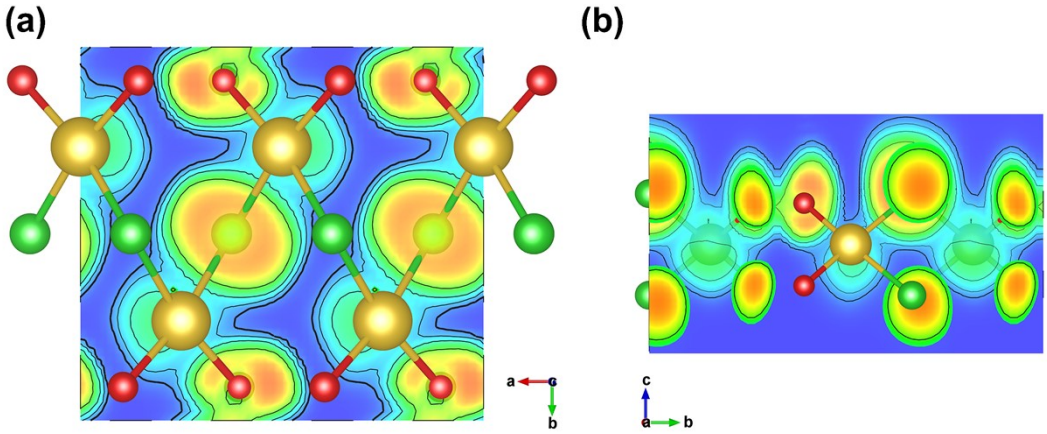

Figure S2. The 2D projected electron location function (ELF) of $AuClO_2$ along (001) and (101) plane visualized by VESTA. The distances from origin are 11 Å (left) and 4 Å (right), respectively.

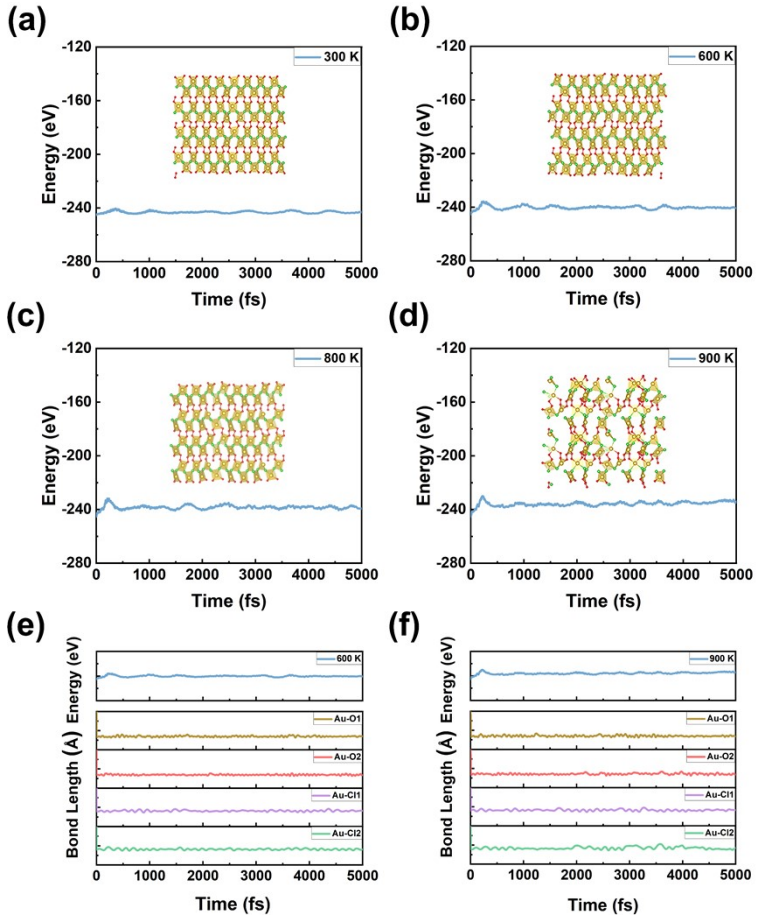

Figure S3. MD simulations of $AuClO_2$. (a)–(d) The total energy fluctuation at 300 K, 600 K, 800 K and 900 K, respectively. Inset: the corresponding snapshots of the structure after 5000 fs. (e)–(f) The bond lengths fluctuation under 600 K and 900 K.

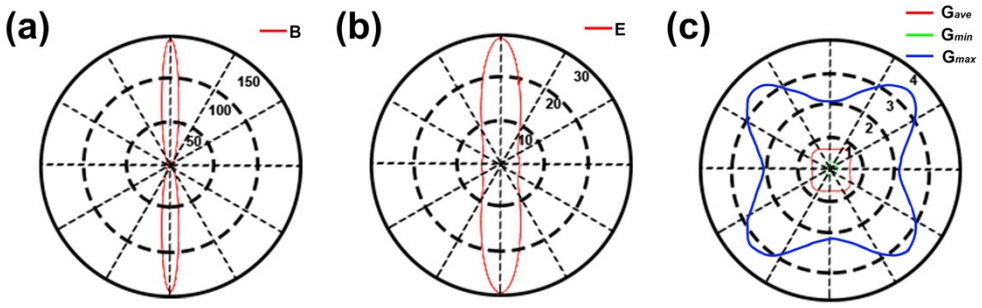

Figure S4. Polar diagrams for (a) Bulk modulus (B), (b) Young's modulus (E), and (c) Shear modulus (G) of $AuClO_2$.

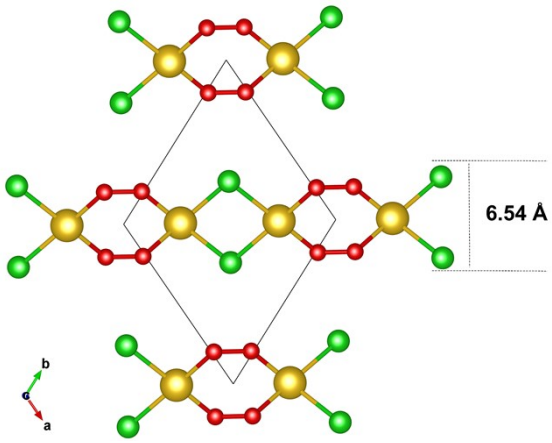

Figure S5. The measured effective thickness of $AuClO_2$ monolayers.

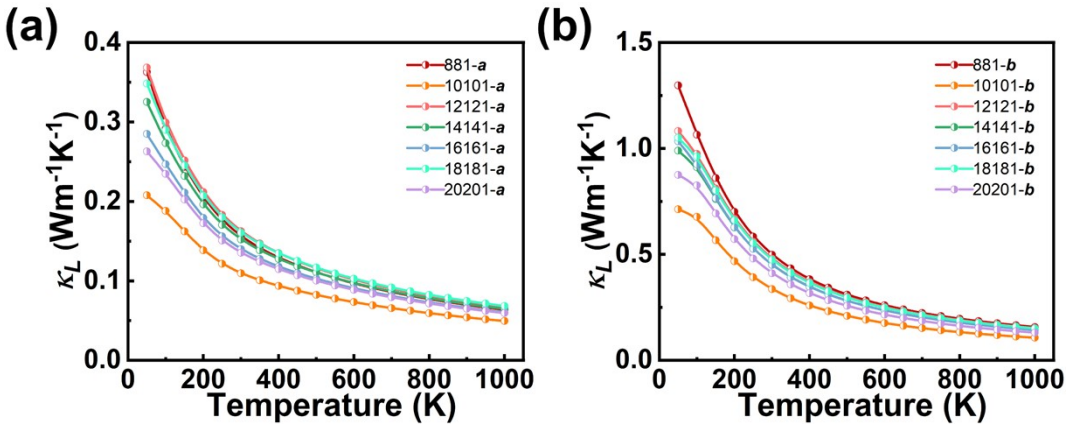

Figure S6. Temperature-dependent κ_L of $AuClO_2$ along the (a) ***a***-axes, and (b) ***b***-axes under different *q*-point mesh.

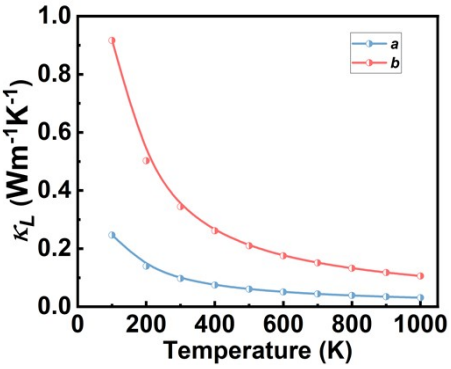

Figure S7. Temperature-dependent κ_L of $AuClO_2$ along the ***a***- and ***b***-axes calculated with the ShengBTE code.

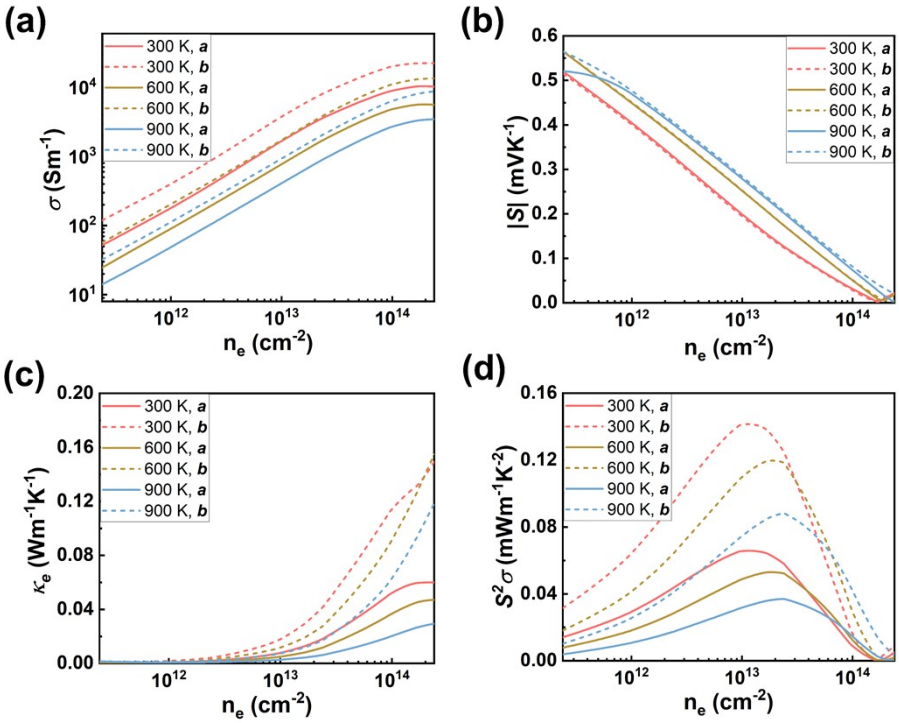

Figure S8. The electronic transport parameters of *n*-type $AuClO_2$ at 300 K, 600 K and 900 K. (a) Electronic conductivity (σ), (b) Seebeck coefficient ($|S|$), (c) Electronic thermal conductivity (κ_e), and (d) Power factor ($S^2\sigma$) along ***a*** and ***b*** axes.

Table S1. The calculated elastic constants (C_{ij}) (GPa), Bulk modulus (B) (GPa), Young's modulus (E) (GPa), and Shear modulus (G) (GPa) for $AuClO_2$.

	C_{11}	C_{12}	C_{22}	C_{33}	B	E	G_{ave}
$AuClO_2$	4.54	2.11	29.86	0.83	2.68	3.78	1.49

Table S2. The Cartesian coordinates of optimized structure $AuClO_2$.

Atom	*x*	*y*	*z*
Au	1.945842147	5.279081563	11.965113640
Au	0.000000000	1.923428318	11.965113640
Cl	2.918763220	3.601254940	13.356273936
Cl	0.972921073	3.601254940	10.573952630
O	1.120960327	0.644329668	10.835441591
O	3.066802590	6.558180105	13.094784975
O	2.770723851	0.644329668	13.094784975
O	0.824881762	6.558180105	10.835441591

References

S1 V. Wang, N. Xu, J.-C. Liu, G. Tang and W.-T. Geng, *Comput. Phys. Commun.*, 2021, **267**, 108033.

S2 S. Tang, M. Wu, S. Bai, D. Luo, J. Zhang and S. Yang, *J. Alloys Compd.*, 2022, **907**, 164439.

S3 A. Togo, Oba, Fumiyasu,Tanaka, Isao, *Phys. Rev. B*, 2008, **78**, 134106.