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Supplementary Materials: Tuning the electronic structure of RhX_3 (X=Cl, Br, I) nonmagnetic monolayers: Effects of charge-injection and external strain†

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In this Supplementary Materials, we present supporting informations regarding the RhX_3 structures, where X=Cl, Br, I.

Here, we present the optimized POSCAR files, including atomic positions and lattice vectors, of RhX_3 structures in cartesian coordinates in Fig. 1, 2, and 3. Ab initio phonon dispersion spectra of related systems under uniaxial and biaxial strain (ε=0.06) are displayed in Fig.4.

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```
RhCl3
1.0
        5.9942998886         0.0000000000         0.0000000000
        0.0000000000        10.3830003738         0.0000000000
        0.0000000000         0.0000000000        23.0000000000
   Rh   Cl
    4   12
Cartesian
     3.007879664         8.652465448         5.590379834
     0.010729797         3.460965571         5.590379834
     3.007939688         5.191500187         5.590149865
     0.010789740         0.000000000         5.590149865
     4.957226115         8.737087328         4.267650098
     1.960076171         3.545586832         4.267650098
     3.909122857         6.922035113         6.913110256
     0.911972824         1.730534616         6.913110256
     4.957345806         5.107086249         4.267650098
     1.960196041        10.298586436         4.267650098
     5.103846796         1.730534616         4.267650098
     2.106696673         6.922035113         4.267650098
     4.055803206        10.298379113         6.912879944
     1.058653261         5.106878617         6.912879944
     4.055683514         3.545483170         6.912879944
     1.058533391         8.736983357         6.912879944
```

Fig. 1 Optimized POSCAR file of monolayer $RhCl_3$

```
RhBr3
1.0
        6.3032999039         0.0000000000         0.0000000000
        0.0000000000        10.9167003632         0.0000000000
        0.0000000000         0.0000000000        24.0000000000
   Rh   Br
    4   12
Cartesian
     3.162806916         9.097322963         5.833199859
     0.011156841         3.638972781         5.833199859
     3.162995896         5.458350182         5.833199859
     0.011345940         0.000000000         5.833199859
     5.217745647         9.177451696         4.412640095
     2.066095695         3.719101514         4.412640095
     4.120593347         7.277727582         7.254240274
     0.968943301         1.819377238         7.254240274
     5.217871508         5.378221448         4.412880063
     2.066221744        10.836571630         4.412880063
     5.356922535         1.819486390         4.412400126
     2.205272583         7.277836897         4.412400126
     4.259959216        10.836462315         7.253999949
     1.108309264         5.378112458         7.253999949
     4.259896097         3.718992199         7.253999949
     1.108246145         9.177342381         7.253999949
```

Fig. 2 Optimized POSCAR file of monolayer $RhBr_3$

```
RhI3
1.0
        6.7743000984         0.0000000000         0.0000000000
        0.0000000000        11.7326002121         0.0000000000
        0.0000000000         0.0000000000        25.0000000000
   Rh    I
    4   12
Cartesian
     3.399275959          9.777244934          6.076249853
     0.012125997          3.910944828          6.076249853
     3.399343794          5.866300106          6.076249853
     0.012193740          0.000000000          6.076249853
     5.605259197          9.867468776          4.547249898
     2.218109148          4.001168670          4.547249898
     4.423888881          7.821772870          7.605999708
     1.036738933          1.955472414          7.605999708
     5.605327032          5.776193750          4.547249898
     2.218176781         11.642493856          4.547249898
     5.761948756          1.955472414          4.546999931
     2.374798707          7.821772870          4.546999931
     4.580578440         11.642258885          7.605750114
     1.193428492          5.775959129          7.605750114
     4.580443174          4.000934049          7.605499774
     1.193292923          9.867233805          7.605499774
```

Fig. 3 Optimized POSCAR file of monolayer RhI_3

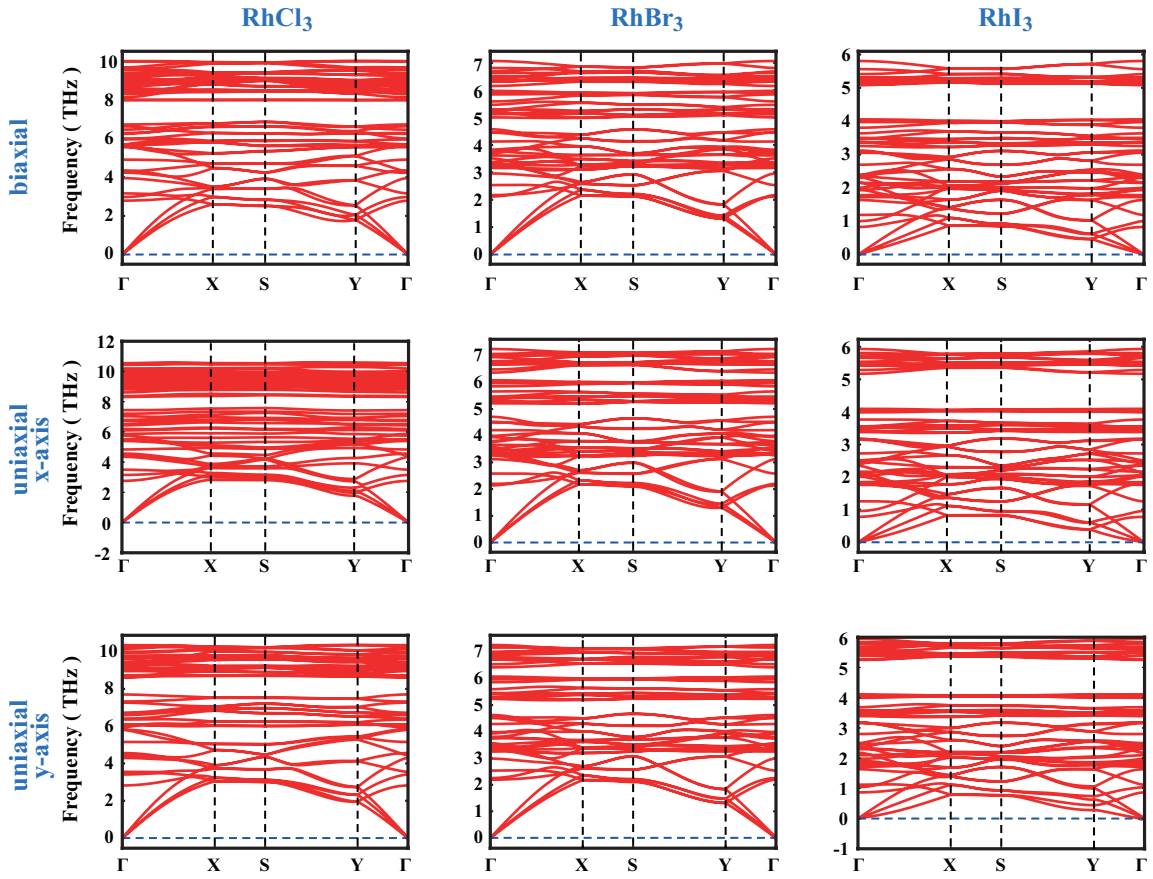

Fig. 4 Ab initio phonon dispersion spectra along the main symmetry directions in irreducible Brillouin zone calculated for optimized $RhCl_3$, $RhBr_3$ and RhI_3 monolayers under tensile strain with the value of ε=0.06.