# Supplementary Information of Role of van der Waals forces in the metal–insulator transition of transition metal oxides

*Da Chen, Quan Ming Li* and Wang Gao**

Key Laboratory of Automobile Materials, Ministry of Education, and School of Materials Science and Engineering, Jilin University, Changchun 130022, China.

**Corresponding Author*email: lqm@jlu.edu.cn,** wgao@jlu.edu.cn**.**

## Structural information

Table S1. Crystal structures of $VO_2$[1, 2]

| Phase | Space group | Lattice parameters (Å, °) | Atom | x | y | z |
|---|---|---|---|---|---|---|
| Metal | $P4_2/mnm$ | $a$ = 4.5546 | V | 0.00000 | 0.00000 | 0.00000 |
| | | $b$ = 4.5546 | O | 0.30010 | 0.30010 | 0.00000 |
| | | $c$ = 2.8514 | | | | |
| Insulator | $P2_1/c$ | $a$ = 5.7517 | V | 0.23947 | 0.97894 | 0.02646 |
| | | $b$ = 4.5378 | O | 0.10616 | 0.21185 | 0.20859 |
| | | $c$ = 5.3825 | O | 0.40051 | 0.70258 | 0.29884 |
| | | $\beta$ = 122.6460 | | | | |

Table S2. Crystal structures of $Ti_4O_7$[3]

| Phase | Space group | Lattice parameters (Å, °) | Atom | x | y | z |
|---|---|---|---|---|---|---|
| Metal | $A$-1 | $a$ = 5.5930 | Ti | 0.21617 | 0.15282 | 0.06282 |
| | | $b$ = 7.1250 | Ti | 0.21852 | 0.65258 | 0.06618 |
| | | $c$ = 12.4560 | Ti | 0.68340 | 0.44002 | 0.20115 |
| | | $\alpha$ = 95.0200 | Ti | 0.68858 | 0.94231 | 0.20136 |
| | | $\beta$ = 95.2100 | O | 0.10730 | 0.86270 | 0.01510 |
| | | $\gamma$ = 108.7300 | O | 0.58700 | 0.79220 | 0.05770 |
| | | | O | 0.85580 | 0.49640 | 0.08110 |
| | | | O | 0.32810 | 0.43850 | 0.13870 |
| | | | O | 0.52650 | 0.14490 | 0.16390 |
| | | | O | 0.03770 | 0.07000 | 0.19810 |
| | | | O | 0.29460 | 0.79050 | 0.79050 |
| Insulator | $A$-1 | $a$ = 5.5900 | Ti | 0.21730 | 0.15600 | 0.06404 |
| | | $b$ = 7.1280 | Ti | 0.21720 | 0.65490 | 0.06596 |
| | | $c$ = 12.4830 | Ti | 0.68160 | 0.44240 | 0.20048 |
| | | $\alpha$ = 95.0300 | Ti | 0.68750 | 0.94250 | 0.19988 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | $\beta$ = 95.3400 | O | 0.10770 | 0.86180 | 0.01560 |
| | | $\gamma$ = 108.8900 | O | 0.58710 | 0.79250 | 0.05670 |
| | | | O | 0.85380 | 0.49670 | 0.08000 |
| | | | O | 0.32330 | 0.44000 | 0.13950 |
| | | | O | 0.52800 | 0.14250 | 0.16590 |
| | | | O | 0.03880 | 0.06910 | 0.19720 |
| | | | O | 0.29250 | 0.78540 | 0.22340 |

Table S3. Crystal structures of $CaFeO_3$[4, 5]

| Phase | Space group | Lattice parameters (Å, °) | Atom | x | y | z |
|---|---|---|---|---|---|---|
| Metal | *Pbnm* | *a* = 5.3263 | Ca | 0.99500 | 0.03280 | 0.25000 |
| | | *b* = 5.3527 | Fe | 0.00000 | 0.50000 | 0.00000 |
| | | *c* = 7.5399 | O | 0.71290 | 0.28580 | 0.03270 |
| | | | O | 0.06630 | 0.49080 | 0.25000 |
| Insulator | $P2_1/n$ | *a* = 5.3118 | Ca | 0.99360 | 0.03710 | 0.25110 |
| | | *b* = 5.3477 | Fe | 0.50000 | 0.00000 | 0.00000 |
| | | *c* = 7.5206 | Fe | 0.00000 | 0.50000 | 0.00000 |
| | | | O | 0.30000 | 0.72000 | -0.03300 |
| | | | O | 0.21900 | 0.20600 | -0.03180 |
| | | | O | 0.07610 | 0.49270 | 0.25400 |

Table S4. Crystal structures of $BaV_{10}O_{15}$[6]

| Phase | Space group | Lattice parameters (Å, °) | Atom | x | y | z |
|---|---|---|---|---|---|---|
| Metal | *Cmca* | *a* = 11.5951 | Ba | 0.00000 | 0.50000 | 0.00000 |
| | | *b* = 9.9458 | V | 0.37110 | 0.40990 | 0.13629 |
| | | *c* = 9.3975 | V | -0.24620 | 0.67110 | 0.11060 |
| | | | V | 0.50000 | 0.67700 | 0.13870 |
| | | | O | 0.12080 | 0.24730 | 0.00100 |
| | | | O | 0.62980 | 0.58850 | 0.24550 |
| | | | O | 0.50000 | 0.34350 | 0.24810 |
| | | | O | -0.25680 | 0.50000 | 0.00000 |
| | | | O | 0.25000 | 0.32430 | 0.25000 |
| | | | O | 0.50000 | 0.50000 | 0.00000 |
| Insulator | *Pbca* | *a* = 11.6120 | Ba | 0.00000 | 0.50000 | 0.00000 |
| | | *b* = 9.8605 | V | 0.50520 | 0.67540 | 0.14150 |
| | | *c* = 9.4149 | V | 0.37470 | 0.41120 | 0.13630 |
| | | | V | -0.24100 | 0.68040 | 0.11200 |
| | | | V | 0.24860 | 0.83010 | 0.60650 |
| | | | V | 0.63440 | 0.09690 | 0.63190 |
| | | | O | -0.25930 | 0.49000 | 0.00100 |
| | | | O | 0.11110 | 0.24800 | 0.00400 |
| | | | O | 0.87270 | 0.25100 | 0.50600 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | O | 0.24100 | 0.32650 | 0.25200 |
| | | | O | 0.63630 | 0.58200 | 0.24300 |
| | | | O | 0.37330 | 0.90500 | 0.74700 |
| | | | O | 0.50500 | 0.34340 | 0.24200 |
| | | | O | 0.50000 | 0.50000 | 0.00000 |

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