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Nearly flat nodal surface states in pseudo-one-dimensional molybdenum monochalcogenides X(MoS)$_3$ (X = K, Rb, Cs)

Tie Yang[1,*] and Xiaoming Zhang[2,*]

[1] School of Physical Science and Technology, Southwest University, Chongqing 400715, China.
[2] School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China.

[*] Correspondence: yangtie@swu.edu.cn; zhangxiaoming87@hebut.edu.cn

Supplementary materials

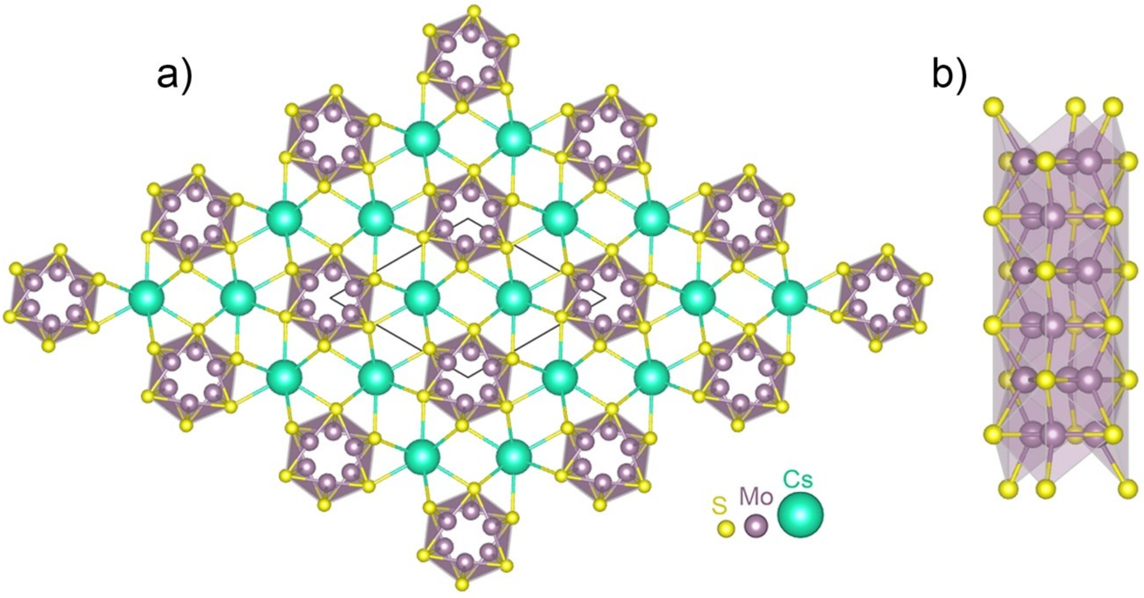

Figure S1: The 2×2×3 supercell structure for Cs(MoS)$_3$ material. a) top view of the structure with Mo atom forming the polyhedral shape. b) side view of a single linear chain clusters formed by a linear condensation of Mo$_6$ octahedral.

In order to properly observe the pseudo-one-dimensional structures of X(MoS)$_3$ (X = K, Rb, Cs) compounds, we take Cs(MoS)$_3$ as an example and draw its supercell structure in Figure S1. The Mo$_6$ octahedral is displayed by the purple color shaded polyhedral shape. We can clearly observe the linear chain clusters (Mo$_3$)1 ∞ distributed evenly in the top view and its side view is shown in Figure S1 b).

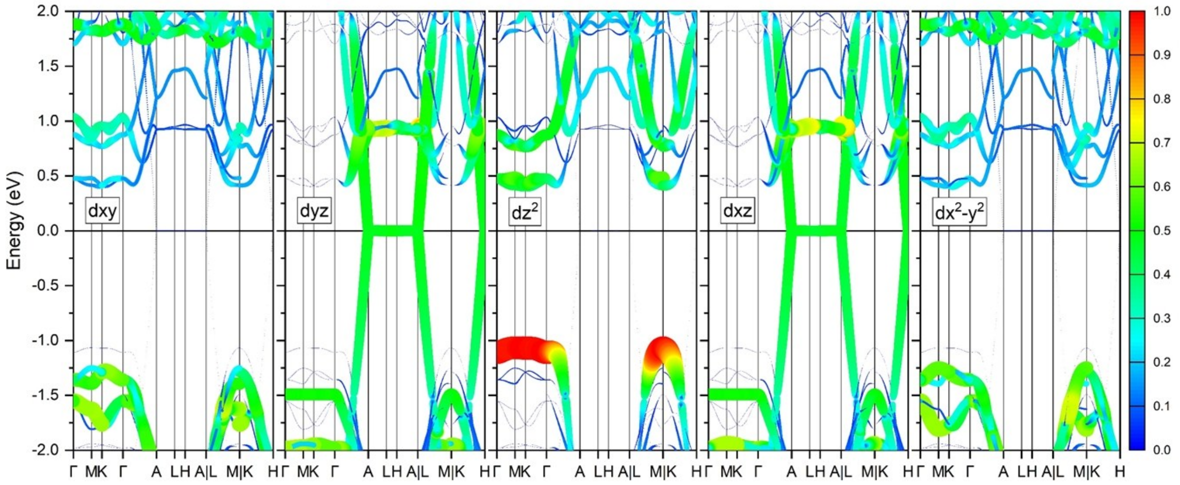

Figure S2: The calculated electronic band structures for $Cs(MoS)_3$ with orbital projections. The projection weight is indicated by the colormap at right side and it is also proportional to the color shade line width.

Through the element weight projection, it is found that the bands near Fermi level are mostly contributed by the Mo element and, especially, the overlap along the A-L-H-A path is completely from Mo element. A detailed orbital decomposition analysis for $Cs(MoS)_3$, as an example, is reported in Figure S2. It is found that flat band overlap mainly has d_{xz} and d_{yz} orbital characters.

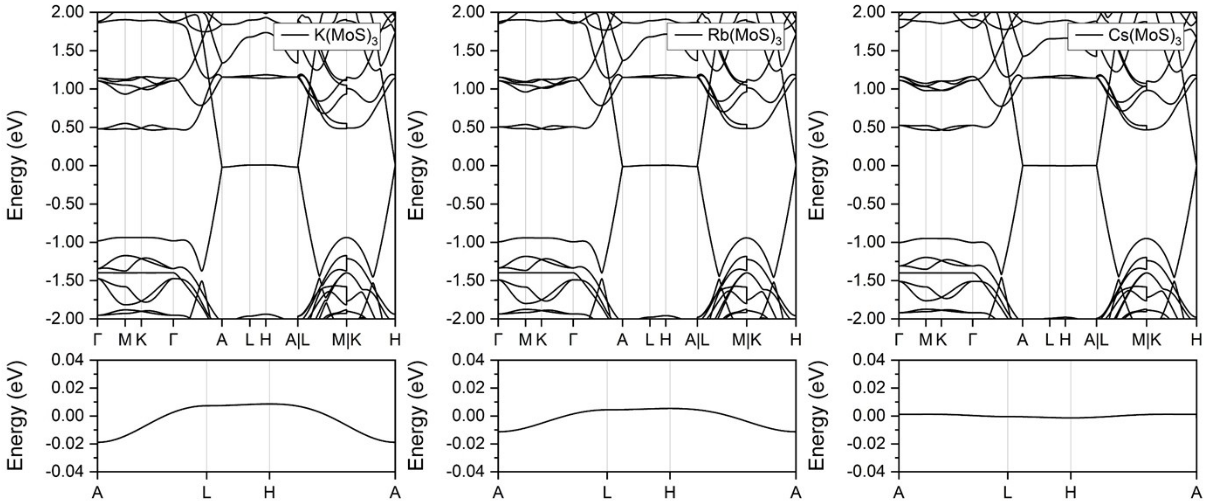

Figure S3: The calculated electronic band structures for $K(MoS)_3$, $Rb(MoS)_3$ and $Cs(MoS)_3$ under DFT+U method. The onsite Hubbard value for Mo is set as 2 eV.

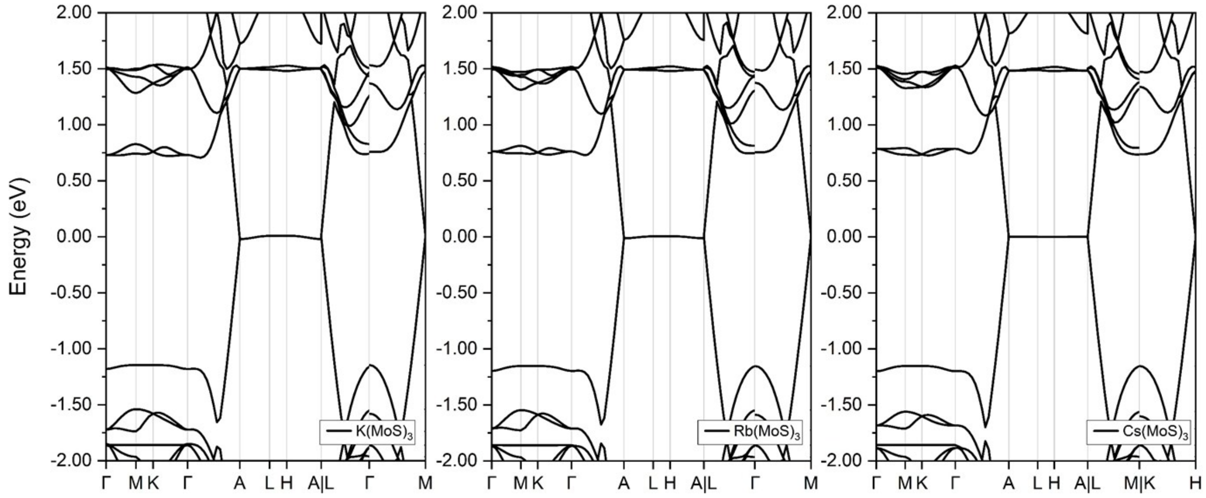

Figure S4: The calculated electronic band structures for $K(MoS)_3$, $Rb(MoS)_3$ and $Cs(MoS)_3$ under HSE06 functional.

Since Mo is a transition metal element, we further apply the DFT+U method and the state-of-the-art Heyd-Scuseria-Ernzerhof (HSE06) functional, which can better deal with the strong correlation effect for its d electrons, to check the band structure, and the obtained band structures are reported in Figure S3 and S4, respectively. It is seen that a similar semimetal signature with band overlap along the A-L-H-A path retained.

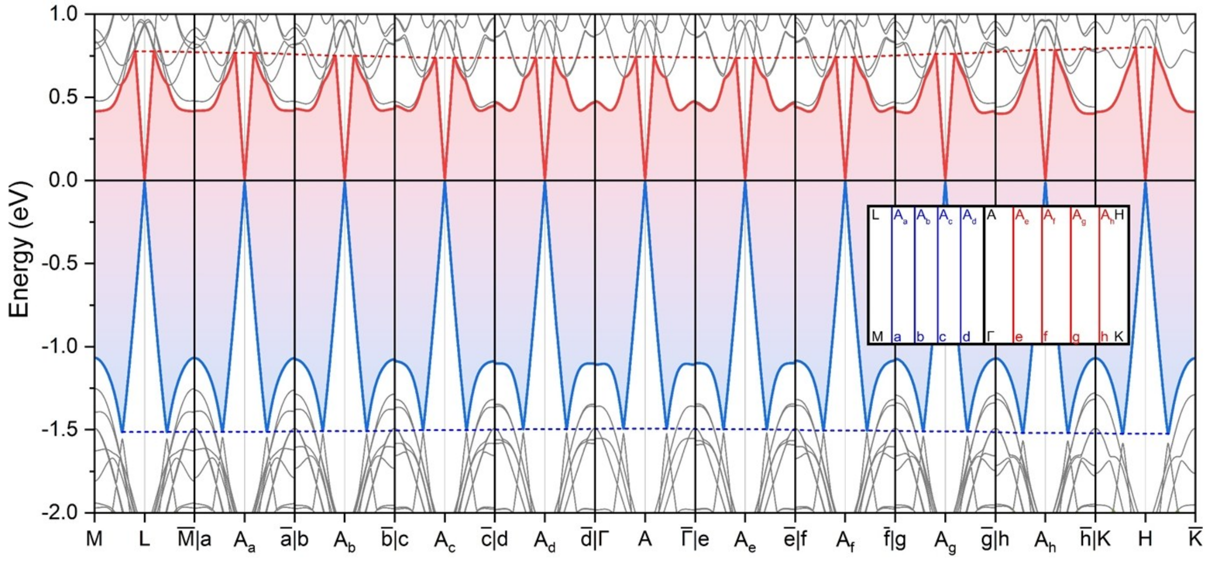

Figure S5: The calculated electronic band structures for $K(MoS)_3$ along different path segments perpendicular to the $k_z = \pi$ plane as indicated in the inset illustration.

A more precise linear dispersion range scan is performed along different path segments perpendicular to the $k_z = \pi$ plane and the obtained results are reported in Figure S5. The linear range maxima and minima along different paths, defined as the lowest maximum and the highest minimum values respectively, are shown in the dash line in the figure. We can see the top/bottom linearity position are all found along the Γ-A path.