

# First-Principles Calculation of MoO<sub>2</sub> and MoO<sub>3</sub> Electronic and Optical Properties Compared with Experimental Data

Eleonora Pavoni <sup>1</sup>, Mircea Gabriel Modreanu <sup>2</sup>, Elaheh Mohebbi <sup>1</sup>, Davide Mencarelli <sup>3</sup>, Pierluigi Stipa <sup>1</sup>, Emiliano Laudadio <sup>1,\*</sup> and Luca Pierantoni <sup>3</sup>

<sup>1</sup> Department of Materials, Environmental Sciences and Urban Planning, Marche Polytechnic University, Via Breccie Bianche, 60131 Ancona, Italy; e.pavoni@staff.univpm.it (E.P.); e.mohebbi@staff.univpm.it (E.M.); p.stipa@staff.univpm.it (P.S.)

<sup>2</sup> Tyndall National Institute, University College Cork, T12 R5CP Cork, Ireland; mircea.modreanu@tyndall.ie

<sup>3</sup> Department of Information Engineering, Marche Polytechnic University, Via Breccie Bianche, 60131 Ancona, Italy; d.mencarelli@staff.univpm.it (D.M.); l.pierantoni@staff.univpm.it (L.P.)

\* Correspondence: e.laudadio@staff.univpm.it

Input geometry of MoO<sub>2</sub>

# Set up lattice

lattice = Monoclinic (5.54483\*Angstrom, 4.87254\*Angstrom, 5.64537\*Angstrom, 90.0\*Degrees, 120.5\*Degrees, 90.0\*Degrees)

# Define elements

elements = [Molybdenum, Molybdenum, Molybdenum, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen, Oxygen, Oxygen, Oxygen, Oxygen]

# Define coordinates

fractional\_coordinates = [[ 0.229730913483, 0.007816652727, 0.213086875905],  
[ 0.229728221644, 0.491773196715, 0.712731710353],  
[ 0.769542910678, 0.991363046157, 0.786202773004],  
[ 0.769545602517, 0.507406502169, 0.286557948549],  
[ 0.111701453446, 0.718438490275, 0.377443761819],  
[ 0.111698761607, 0.780331058051, 0.877088586274],  
[ 0.887575062554, 0.218848640833, 0.122201062636],  
[ 0.887572370715, 0.280741208609, 0.62184588709 ],  
[ 0.390349418272, 0.197725282573, 0.591309054382],  
[ 0.390352110111, 0.301864566869, 0.091664229928],  
[ 0.60892171405 , 0.697315132015, 0.907625418981],  
[ 0.608924405889, 0.801454416311, 0.407980594527]]

Input geometry of MoO<sub>3</sub>

# Set up lattice

lattice = Orthorhombic (3.909\*Angstrom, 13.855\*Angstrom, 3.68131\*Angstrom, 90.0\*Degrees, 90.0\*Degrees, 90.0\*Degrees)

# Define elements

elements = [Oxygen, Oxygen, Molybdenum, Oxygen, Oxygen, Oxygen, Oxygen,  
Molybdenum, Oxygen, Oxygen, Molybdenum, Oxygen, Oxygen, Oxygen,  
Oxygen, Molybdenum]

# Define coordinates

fractional\_coordinates = [[ 0.037785290332, 0.137982542827, 0.000000227662],  
[ 0.548288252624, 0.189282496069, 0.500000257704],  
[ 0.507387648141, 0.309244274572, 0.500000320919],  
[ 0.06540607799 , 0.324759633975, 0.50000025144 ],  
[ 0.585348864739, 0.34763758581 , 0.000000262578],  
[ 0.584659258008, 0.479104281039, 0.500000217995],  
[ 0.104682870799, 0.502068181388, 0.000000208718],  
[ 0.66198538547 , 0.5173553747 , 0.000000189186],  
[ 0.615418711333, 0.637239874338, 0.000000241267],  
[ 0.106979591451, 0.690072960965, 0.500000226912],  
[ 0.147767493255, 0.810064791932, 0.500000128325],  
[ 0.589546057794, 0.826275592252, 0.50000019184 ],  
[ 0.069135486408, 0.848324778092, 0.000000174242],  
[ 0.068472360777, 0.979844330377, 0.500000216522],  
[ 0.548313826659, 1.002687042621, 0.000000229065],  
[-0.00933012138 , 1.018047094926, 0.000000176113]]