

Perovskenes: Two-dimensional perovskite-type monolayer materials predicted by first-principles calculations (Supplementary)

Mosayeb Naseri^{1,2*}, Shirin Amirian², Mehrdad Faraji³, Mohammad Abdur Rashid⁴, Maicon Pierre Lourenço⁵,
Venkataraman Thangadurai⁶, D.R. Salahub^{1*}

¹Department of Chemistry, Department of Physics and Astronomy, CMS – Center for Molecular Simulation, IQST –
Institute for Quantum Science and Technology, Quantum Alberta, University of Calgary, 2500 University Drive
NW, Calgary, Alberta, Canada, T2N 1N4

²Department of Physics, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

³Micro and Nanotechnology Graduate Program, TOBB University of Economics and Technology, Sogutozu
Caddesi No 43 Sogutozu, 06560 Ankara, Turkey

⁴Department of Physics, Jashore University of Science and Technology, Jashore 7408, Bangladesh

⁵Departamento de Química e Física – Centro de Ciências Exatas, Naturais e da Saúde – CCENS – Universidade
Federal do Espírito Santo, Alegre, Espírito Santo, Brazil

⁶Department of Chemistry, University of Calgary, Calgary, Alberta T2N 1N4, Canada

*To whom correspondence should be addressed.

Email addresses: mosayeb.naseri@ucalgary.ca (M. Naseri) dsalahub@ucalgary.ca (D.R. Salahub)

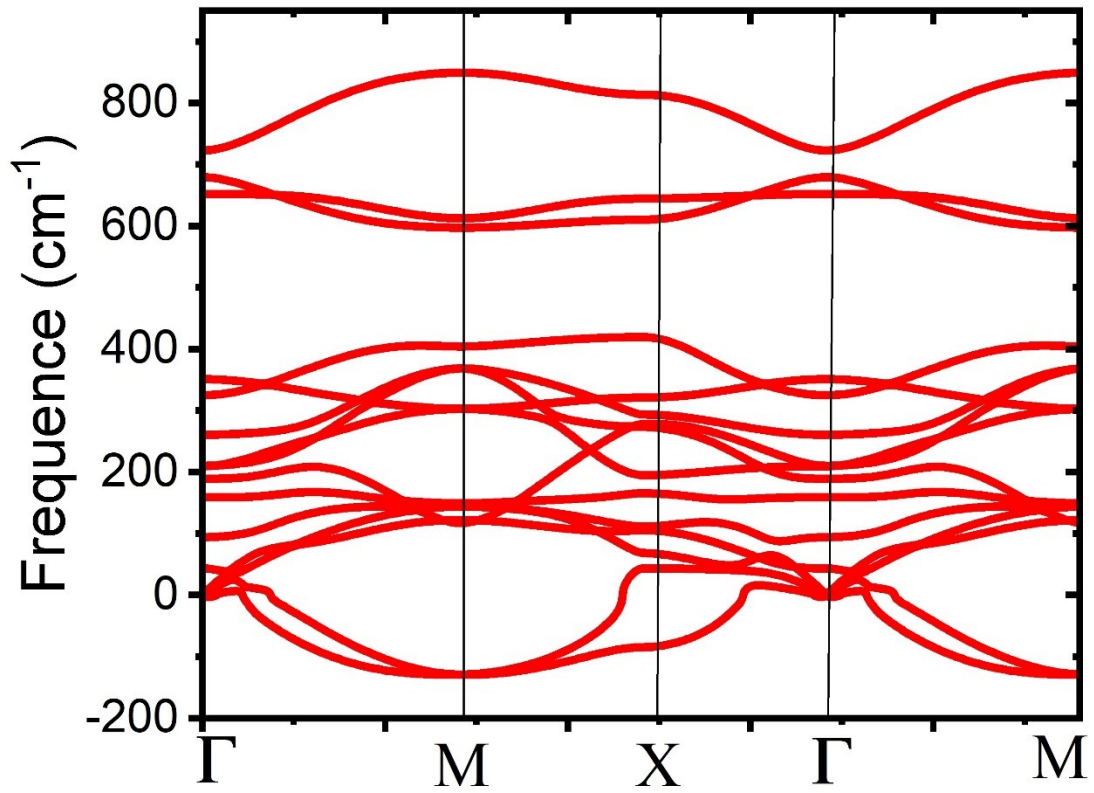


Figure S1: Phonon dispersion modes for 2D SrZrO3 monolayer.

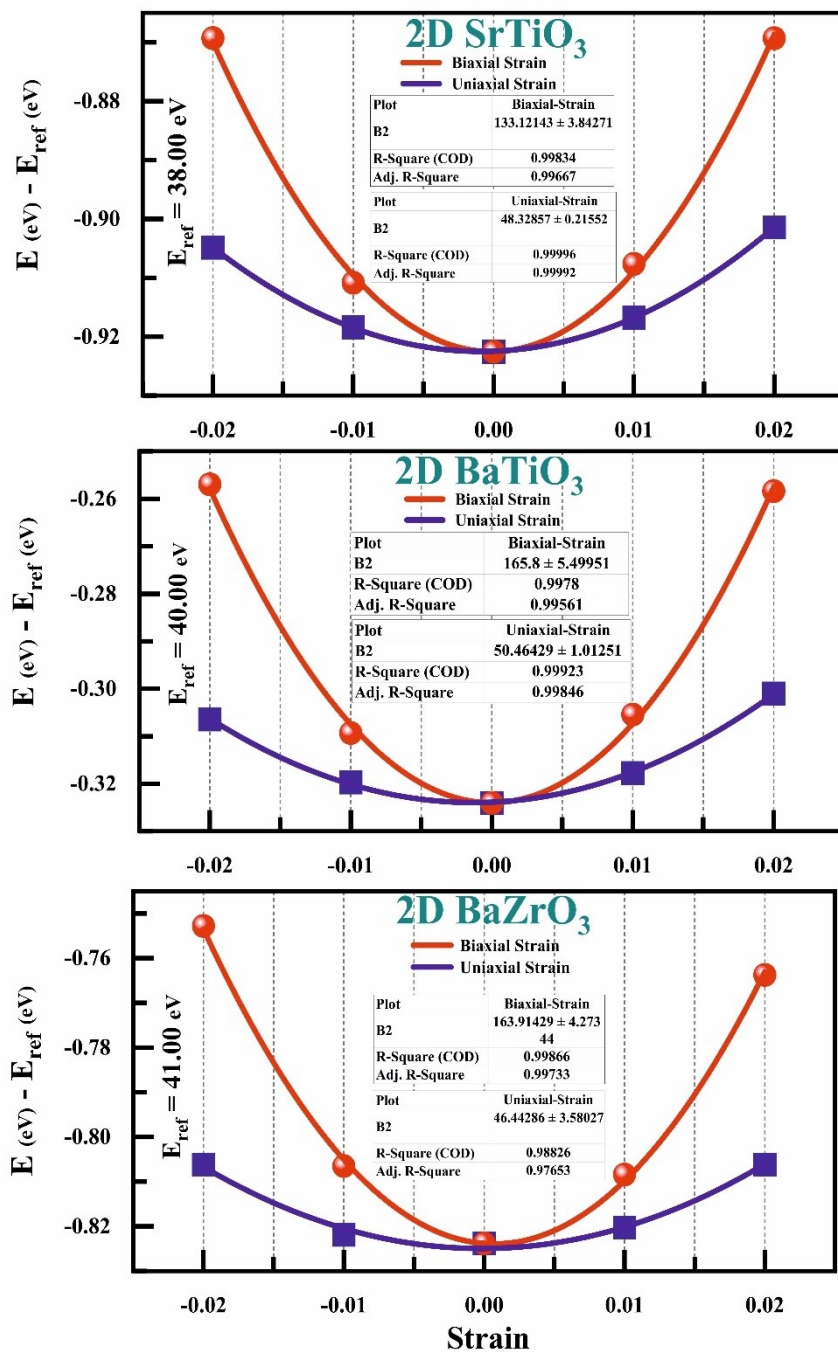


Figure S2: The variation of strain energy of the 2D SrTiO3, BaZrO3 and BaTiO3 monolayers under biaxial and uniaxial strains.

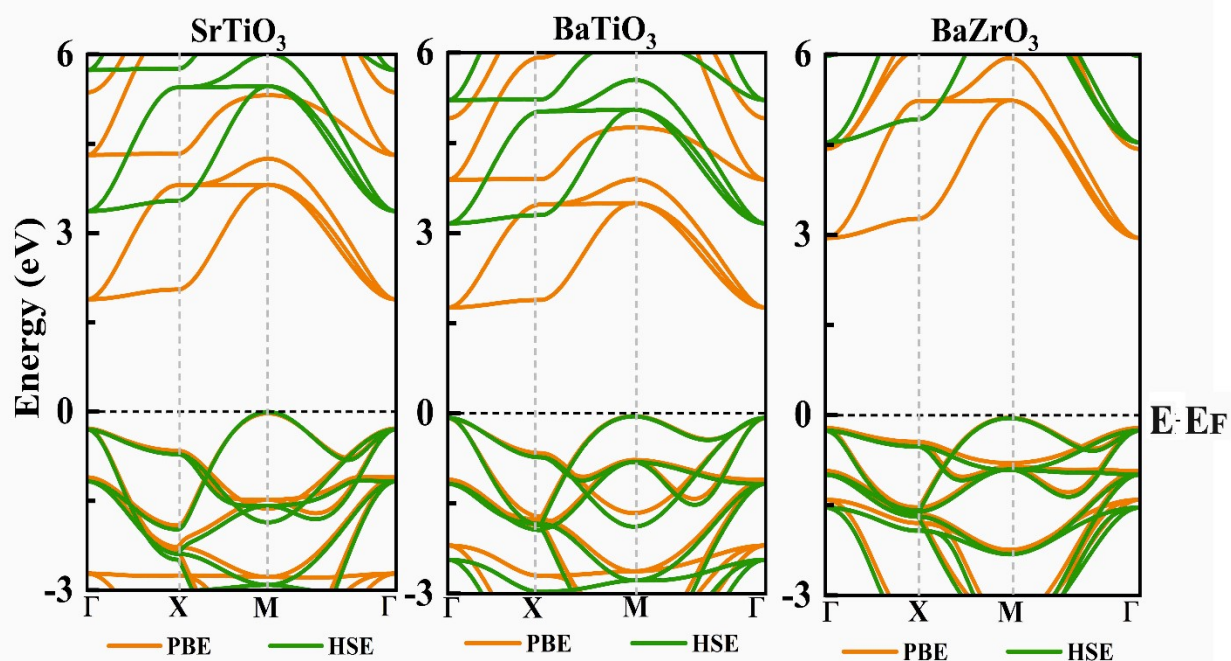


Figure S3: Band structures for SrTiO_3 , BaTiO_3 and BaZrO_3 perovskites calculated by PBE and HSE06 levels of theory.