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An ab initio density functional theory study of structural, electronic, magnetic and optical properties of Niobium diphosphide (NbP2)

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Abstract content
   (Max 300 words)
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One of the fascinating things about numerical simulations of properties of materials is that it helps predict and explore materials ranging from those whose properties have already been established experimentally to those that are yet to be explored. In this study, we report structural, electronic, magnetic and optical properties of Niobium diphosphide which have not been reported before. We confirm that NbP2 in the C 1 2/m 1 structure is energetically, mechanically and dynamically stable. It is a metal, but in contrast to Niobium chalcogenides it is not magnetic. Optical properties are explored at the Density Functional level of approximation as well as at the GW and BSE approximations of many-body perturbation theory.

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 (Hons, MSc,
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Msc

Main supervisor (name and email)
and his / her institution

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