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Prediction and Mechanical Characterization of the Al-P compounds by ab-initio Minima Hopping O. PALVIC, I. VALENCIA-JAIME, West Virginia University, A.C. GARCIA-CASTRO, CINVESTAV-Queretaro, A.H. ROMERO, West Virginia University — The III-V group compound semiconductors, including GaAs and InP, have led to large technological advances [1]. Of these, AlP has the largest direct band gap (3.56 eV) and is arguably the least understood [2]. Here, we present a study of the AlP phase-diagram by means of first principle minima hopping calculations [3]. We were able to reproduce the previously obtained structure for AlP (cubic, F-43m). Also reported here are a large number of metastable structures and the mechanical properties as a function of the P content. We discuss alternative path for synthesis to stabilize metastable structures. Our results are relevant also for ternary alloys such as AlInP, AlAsP, and AlPSb. Such compounds have applications in quantum wells [4], solar cells [5], and optical equipment [6]. Our research is the initial step for the ternary characterization.

[1] New Supercomputers use GaAs Technology. Mechanical Engineering 116.8(1994):10
[2] I. Vurgaftman, J of App Phys 89(11),5828(2001)
[3] S. Goedecker, The J of chem phys 120,9911(2004)
[4] Ishitani et al. J of App Phys 80.8 (1996):4592.
[5] I.A. Morozov, A.S Gudovskikh. Semiconductors 48.4,459-64(2014)
[6] Shimomura, H; Anan, T; Sugou, S. Seventh International Conference on Indium Phosphide and Related Materials,1995,ISBN 9780780321472,801-804

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