A comparative study of Ag doping effects on the electronic, optical, carrier conversion, photocatalytic and electrical properties of MoS_2(Article)

- Kamruzzaman, M.,
- Zapien, J.A.,
- Afrose, R.,
- Anam, T.K.,
- Rahman, M.,
- Liton, M.N.H.,
- Helal, M.A.,
- Khan, M.K.R.,
- Ayotunde Emmanuel, A.
- View Correspondence (jump link)
- [a]Department of Physics, Begum Rokeya University, Rangpur, Rangpur, 5400, Bangladesh
- [b]Department of Materials Science and Engineering and Center of Super-Diamond and Advanced Films (COSDAF), City University of Hong Kong, Hong Kong
- [c]Department of Textile Engineering, Uttara University, House-7, Road-16, Sector-4, Dhaka, 1230, Bangladesh

View additional affiliations

Abstract

MoS_2 is an interesting material due to its intriguing properties and potential applications. Theoretical and experimental studies demonstrated p-type of Ag doped MoS_2 system. Band structures, density of states and I-V characteristics confirmed that Ag is an efficient acceptor and indirect band gap is reduced with Ag doping. Formation energy is negative which indicates the substitution reactions could be possible. MoS_2 is a strong photocatalyst for O_2 production and the oxidation ability is enhanced with Ag doping. $Mo_{100-x}Ag_xS_2$ (x = 0.0 to 10) thin films seems to be stacked of many layers and XRD patterns justify hexagonal crystal structure. EDX and XPS measurements ensured the films are composed of Mo, S and Ag. Rectification is observed for Au/$Mo_{100-x}Ag_xS_2$ and the forward current decreases with Ag. The built-in potential is just opposite side to undoped MoS_2 insights p-MoS_2. Thus Ag doped MoS_2 would enable for fabrication of efficient electronic, photocatalytic and optoelectronic devices. © 2021

Author keywords

DFTFormation energyIndirect-direct band gapp-type MoS_2PhotocatalyticXPS

Indexed keywords

Engineering controlled terms:	Crystal structureEnergy gapLayered semiconductorsMolybdenum compoundsOptoe devicesSemiconductor dopingSilverSubstitution reactions
Engineering uncontrolled terms	Ag dopedAg dopingComparatives studiesDFTDirect band gapFormation energiesInd typeP-type MoS2Photo-catalytic
Engineering main heading:	X ray photoelectron spectroscopy

Funding details

- Funding text

This work was supported by a grant from the Begum Rokeya University , Rangpur, Ragpur-5400, for fiscal year 2018-2019, Bangladesh.

- **ISSN:** 09215107
- **CODEN:** MSBTE
- **Source Type:** Journal
- **Original language:** English
- **DOI:** 10.1016/j.mseb.2021.115442
- **Document Type:** Article

- **Publisher:** Elsevier Ltd