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# Electronic Structure and Optical Properties of Oxygen Vacancy and Ag-Doped $SnO_2$ Sensors

Yong Li[a,b], Yuxin Zhang[a], Shiqiang Cui[b], Yaping Ding[*c], Jiyu Tang[d], Ruizhu Zhang[a]

[a]Dept.of Mechanical Engineering, North China University of Water Resources and Electric Power, Zhengzhou, 450046, China
[b]School of Materials Science and Engineer, Shanghai University, Shanghai, 200444, China
[c]Department of Chemistry, Shanghai University, Shanghai, 200444, China
[d]School of Materials Science and Engineering, Zhengzhou University, Zhengzhou, 450001, China
wdingyp@sina.com

Crystal structure, electronic and optical performance of oxygen vacancies defects and Ag-doped were calculated for $SnO_2$ (rutile) semiconductor. In this paper, the examines were accomplished electronic structure, band structure, parity density of state and optical properties by first-principle, in order to demonstrate the crystal stability and the change of electronic structure due to different concentration of vacancy, and to investigate the distribution of PDOS with different concentration of Ag-doped based on draw guide width, band gap, Fermi-level changes and the distribution of the absorption spectra. The results showed the phenomenon including electron localization levels and narrow band gap and red shift of the absorption spectrum. Moreover, indicated that oxygen vacancies and Ag-doped $SnO_2$ can better improve conductivity. In addition, our investigation further revealed that the optical absorption capacity enhanced with increasing the electronic and optical properties in $SnO_2$ internal situation, which should improve the photocatalytic performance, and provide more valuable instructional information for designing new sensor materials.

## 1. Introduction

Gas sensitive sensors are focused on improving the sensitivity and stability and selectivity, and expanding the scope (Kim et al., 1999, Hays et al., 2005 and, Rajpure et al., 2000), therefore, chemical sensors have gained consideration attention in environmental monitoring. Recently, $SnO_2$ as a broad-spectrum gas material is widely regarded as a transparent conductor and sensor materials due to excellent optical and electrical properties, and thus Tin dioxides hold great promise for applications as semi-conductors (Hartnagel et al., 1995 and Look et al., 2004). Currently, Tin dioxide has been already used in sensors, solar cells, photovoltaic devices, spintronic devices and transparent conductive electrode, et al. (Kim et al., 2011; Snaith and Ducat, 2010; Liu et al., 2007; Zhang and Chen, 2015; Borges et al., 2012; Lewis and Paine, 2000). Especially, $SnO_2$ as a kind of functional materials is owing to material composition, microstructure and the catalytic activity of the surface modification of doping, etc., which is the key factor of gas sensor performance used in transparent conductive film of ownership (TCO) and chemical gas sensors. However, literature on optical properties is little information, and the mechanism of photoluminescence is inconclusive. Hence this paper was mainly concerned on investigation of $SnO_2$ (rutile) semiconductor.

Through $SnO_2$-based gas sensor has low sensitivity and poor stability, some technologies including surface modification, surface doping, catalytic layer and nano materials can improve the detection ability (Abhijit et al., 2015; Li et al., 2016; Dhanya et al., 2015). Reports advocated showed that oxygen vacancies and doping are useful for conductivity of $SnO_2$, which is due to the REDOX reaction between sensitive material and gas measured, so that sensitive degree is different because of doping and testing temperature. Then studies (Baraneedharan et al., 2015; Sun et al., 2008; Dhanya et al., 2015; Qin et al., 2009) further demonstrated that the concentration of a specific gas can accurately detect from variety mixture ingredients by controlling the crystal defects and doping. Similarly, the same to other semiconductor materials, appropriate element doped in $SnO_2$ may significantly affect the more sensitive feature, in addition, the response and recovery time of

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performance can be further improved. Respectively, a lot of experiments and theory works were focused on different elements doped $SnO_2$ system to discuss electronic structure(Giuseppe et al., 2016 ) and optical properties. More recent examines reported the exploration of electronic and optical properties of Ag doped in $SnO_2$ (Liu et al., 1997). In fact, Ag doped due to the unique properties of photocatalytic ability is considered to be great significance for industrial application prospect of a mixed material.

At present, there is little information available in literature on the system of Ag doped $SnO_2$, and the discussion of doping distribution and defects has not agreed on consensus. So quantum chemical calculations were carried out into these issues via first-principles calculations(Wang et al., 2015) and based on density functional theory (DFT) ( Hohenberg and Kohn, 1964), and it may provide a good prediction coupled with molecular dynamics (Benedek et al., 1999; Tang and Holzwarth, 2003; Sigala et al., 1995; Yong et al., 2015; Rossi et al., 2015). Furthermore, considerable theoretical experiments have been devoted to the phase structure, electric and optical properties of $SnO_2$ (Scanlon and Watson, 2012; Schleife et al., 2013). In this paper, there are two aspects of these issues to be addressed, the first question related to different concentration of oxygen vacancies, and the second problem deal with different concentration of Ag-doped. In order to investigate electronic and optical properties through calculating band structure, parity density of states, Fermi-level changes and the distribution of the absorption spectra, so as to improve the absorption properties and make the precision of calculation and guarantee the accuracy of the calculation results. As a consequence, investigation was implemented in the Castep package to provide theoretical and experimental guidance for the design a new generation of sensors materials.

## 2. Methods and Computational Details

Firstly, the convergence of calculation relied on structural model optimized via first principles**(**Triki and Ezzeddine, 2008**),** and set the appropriate parameters including density approximation function and plane wave basis set extensions in the framework, and the exchange-correlation part is described with generalized gradient approximation (GGA) (Perdew et al., 1993) and projector augmented wave (PAW) potentials and the perdew burke ernzerhof (PBE) (Perdew et al., 2006; Hammer et al., 1999), and the exchange-correlation function was used to describe under the spin-polarized. As well-known, $SnO_2$ (rutile) is a wide band-gap and n-type semiconductor material for transparent electrodes (Dawar et al., 1995), and its space group is the P42/mnm, and then Pseudopotentials (Ravindran et al., 1998) of electronic calculation executes norm-conserving (Hartnagel et al., 1995). Additionally, $SnO_2$ can be simplified as a set of face-centered cubic lattice, and its symmetry is D4h-I4 with lattice constants. Namely, Sn atoms occupy the position of vertices and body-centered of tetragonal body in $SnO_2$ unitcell, and O atoms form a distorted hexagonal packing, moreover, each crystal cell is composed of six atoms (two Sn atoms and four O atoms).

In view of convergence, interatomic force is less than $0.03eVnm^{-1}$, and the maximum forces on each relaxed atom is less than $1\times10^{-6}eV\cdot atom^{-1}$. Respectively, internal stress is lower than 0.05GPa, and the lattice parameters and the atomic position are fully relaxed. According to the Monkhorst-Pack scheme (Monkhorst et al., 1976) k-point mesh with 5×5×8 (for unitcell cases) used for the integration of the Brillouin zone, energy calculate in reciprocal space under the condition of periodic boundary conditions. When band gap was in converged value 3.6eV (Shieh et al., 2006; Dawar and Joshi, 1984; Dean J. A. (ed.), 1992), $E_{cut\text{-}off}$ (Cut-off Energy) for the plane waves is chosen to 400eV. In this case, $SnO_2$-doped materials are prepared to improve the electrochemical properties, and further guide the design and synthesis of $SnO_2$-based materials with the higher performance.

*Table 1: Structural parameters between optimized calculation and experiment of $SnO_2$*

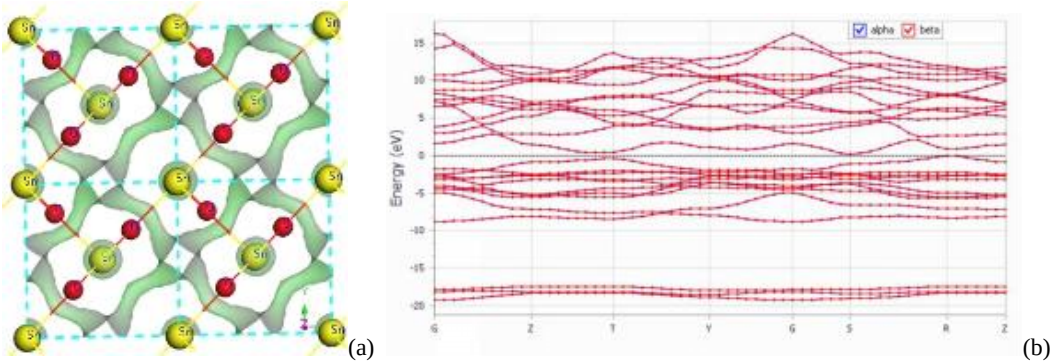
| Parameters | Experiment | Calculation |
|---|---|---|
| a/Å | 4.7370 | 4.8902 |
| b/ Å | 4.7370 | 4.8902 |
| c/ Å | 3.1860 | 3.2854 |

Generally, crystal structures of $SnO_2$ contain oxygen vacancy or Tin-ion, and generate free electrons due to the presence of $O_2$-space and doping. Therefore, supercell (2×2×2, $Sn_{35}O_{40}$) was built according to oxygen vacancy defects and Ag miserably impurity of $SnO_2$ system. Furthermore, in consideration of oxygen vacancy, the crystal system keeps electrically neutral because O atoms was removed, and the work respectively established $Sn_{35}O_{32}$ (oxygen vacancy concentration 10.67%, and similar hereinafter), $Sn_{35}O_{24}$ (21.33%) and $Sn_{35}O_{12}$ (37.33%). On the contrary, Ag atoms in the crystal structures of Ag doped was replaced by one or more Sn atoms, so experimental established $Sn_{34}Ag_1O_{40}$ (1.33%), $Sn_{27}Ag_8O_{40}$ (10.67%) and $Sn_8Ag_{27}O_{32}$ (36.00%). In addition, calculation of all the electronic structure and optical properties relied heavily on crystal

geometry and structure optimization, which made all the atoms of the supercell fully relaxed. Consequently, the shape (mainly noted side length) of model optimized was changed, and optimized results and the experimental results are shown as Table 1. Both data of theory and numerical (Hartnagel et al., 1995; Singh et al., 2008; Anderson et al., 2011) were very similar, which implied the precision theoretical calculation, and also indicated the reliable model calculated. Although the cell dimensions were not enough to reach the size of the test scenario, calculations reflected the typical Ag-ion doping concentration and described correctly interactions of the Ag-Ag.

## 3. Results and Discussion

In this study, the effects of vacancy and Ag-doped with different concentration were investigated by first principles, and electronic structure, band structure, PDOS and absorption spectra were mainly examined. Noted that density of $SnO_2$ around vacancy changed when one O atom is removed from lattice of $SnO_2$ semiconductor, and then its structure remain two electrons in the structure in order to keep space charge neutral. Simultaneously, oxygen vacancy being positively charged center has the attractive potential of negative coulomb, and the conduction band energy moved to the low energy and became donor level into the band gap formation, additionally, it is clear that the energy locates in the higher energy range (-8.97eV~0eV) and low energy range (-19eV~-16.5eV). As a result, valence band across the Fermi surface into band gap in view of Figure 1, and conduction band also move to relatively low energy direction. Moreover, the movement is more obvious. At the same time, excess electrons in crystal lattice may transfer $Sn^{4+}$ into $Sn^{3+}$ (Yang et al., 1995). Although some $Ag^{+}$ ion can enter the lattice, it is difficult for $Ag^{+}$ ion to replace $Sn4^{+}$ ion. Consequently, one difficulty is a silver oxide molecules separate three oxygen vacancies, the other is the radius of $Ag^{+}$ greater than $Sn^{4+}$, thereby, lattice distortion is caused.




(a) (b)

*Figure 1: Electronic structure (a) and band gap of $Sn_{35}O_{32}$ (b)*

In theory, $SnO_2$ belongs to the typical insulators, but the chance of one electron guided its valence band is tiny on account of existing oxygen vacancy in room temperature. Then experiment further demonstrated that conduction of $SnO_2$ semiconductor is not heavily dependent on intrinsic excitation but additional energy level of electrons or holes on the excitation, namely the donor level electronic or acceptor level hole, which indicated that oxygen vacancy can play free electron ionization caused by tin oxide show n-type (Çetin and Alex, 2002; Godinho et al., 2009) semiconductor material properties.

Figure 2 shows PDOS diagram of $SnO_2$ structures with different concentration of oxygen vacancy, and the narrow energy gap and indirect band gap could dramatically enhance the photocatalytic properties. Therefore, calculation results suggested that oxygen defects were composed of Sn-gap and O-space, and remained the defect into the energy gap and then make the band gap narrowing ratio compared to pure Tin oxide. Moreover, different ratios of oxygen vacancies experiment showed that electronic structure of $SnO_2$ changed with different doping concentration of oxygen vacancy, but also conductivity was better than pure $SnO_2$ after losing O atoms, and the materials with vacancy easily absorbed the reducing gas. In addition, the stability of $SnO_2$ crystal decreased, and the deformation of the whole structure was also increased with concentration increased of oxygen vacancy. Although the symmetry declined, the whole lattice still belongs to rutile structure.As for influence on the electrical conductivity of Ag doped, calculation took account of substitutional doping effect of $SnO_2$ (rutile). In this paper, the supercell (2×2×2) was calculated using impurity atoms to take place of Sn atoms, and in order to test the feasibility of Ag doped inside crystalline. Accordingly, in consideration of reducing the impact of border effects, the work firstly selected one Ag atoms to replace Sn atoms in the center position, and then named $Sn_{35}Ag_1O_{40}$, and further increasing the doping concentration to form different supercell ($Sn_{27}Ag_8O_{40}$ and $Sn_8Ag_{27}O_{40}$).

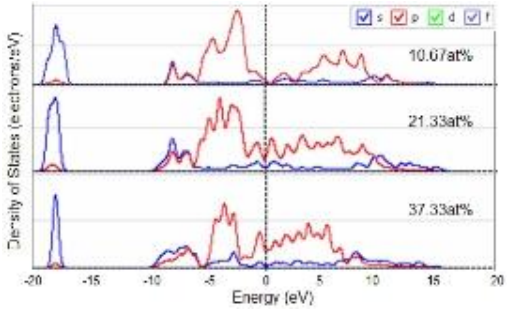
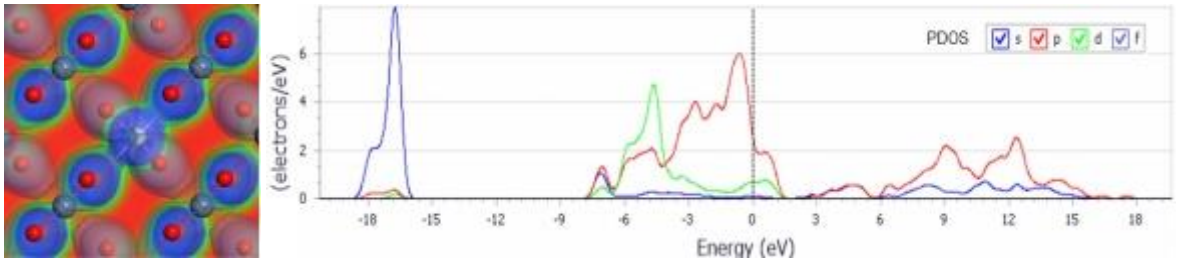



*Figure 2: PDOS with different concentration of oxygen vacancy*




a- structure of $Sn_{35}Ag_1O_{40}$ b-PDOS of $Sn_8Ag_{27}O_{40}$

*Figure 3: Electrical structure and PDOS with different concentration of oxygen vacancy*

Subsequently, the result of electrical structure and PDOS is shown in Figure 3a, 3b, and showed that band gap becomes smaller and makes Fermi level across the band after Ag doping. Figure 3b shows that it is difficult to determine band gap. The explanation was to emerge several layers of narrow electronic states at the top and bottom of valence band, and then make the guide width narrowing. However, conduction band at the bottom takes place large movement down, which led to the band gap becomes smaller. Furthermore, the valence band electrons are excited into the conduction band and excitation energy required is also reduced, which can cause a red shift phenomenon. In addition, the valence band near the top emerged a significant peak of DOS, which may also cause the absorption spectra of $SnO_2$ moving towards the longer wavelength region. According to the theory of semiconductor doping in degenerate semiconductors, the function of impurity band is useful to improve the photocatalytic activity of $SnO_2$.

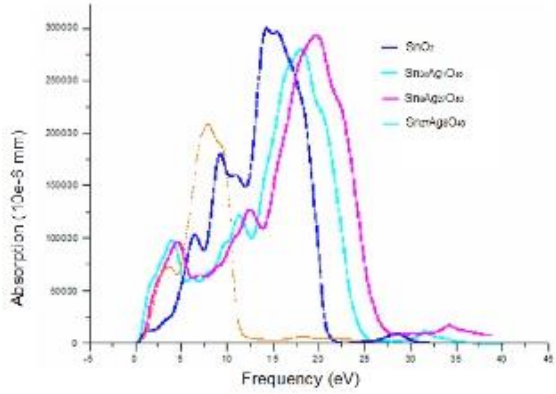



*Figure 4: Absorption spectra of pure $SnO_2$ and Ag doped $SnO_2$*

Finally, the transparency of Ag doped $SnO_2$ films prepared at different oxygen flow rate has been investigated**,** in order to examine the effects of Ag doped $SnO_2$ on optical absorption properties. Figure 4 shows that the maximum of absorption peak with different doping concentration is from $2.1\times10^2 mm^{-1}$ to $2.9\times10^2 mm^{-1}$, and the studies calculated absorption spectra of pure $SnO_2$ and Ag doping different concentration. Compared without Ag doped $SnO_2$ (rutile), certain degree red shift of absorption band appeared because of impurity

atoms. Moreover, in the light of Ag doping impurities, the corresponding optical absorption gradually shifted to a longer wavelength region. When doping concentration was 10.67%, the effect of light absorption was best, and Figure 4 shows that Jane band formed between 4d impurities band of Ag doped and conduction. Furthermore, electrons could easily transmit from valence band to conduct band with decreasing width of band gap. In consequence, absorption capacity could be obviously enhanced in the lower energy areas. Compared with other works and results, it should be noted that this study has examined optical performance only with first-principles calculations. Notwithstanding its limitation, this work suggests to investigate optical absorption with more elements doped $Sno_2$ to improve the catalytic performance.

## 4. Conclusions

In summary, in view of oxygen vacancies defects and Ag-doped, the investigation demonstrated electronic structure, band structure and PDOS of $SnO_2$ in the rutile, and indicated band gap, Fermi-level changes and the distribution of the absorption spectra of pure $SnO_2$ and Ag doped $SnO_2$ via first principles. Obviously, the results show that the phenomenon including electron localization levels and narrow band gap and red shift of absorption spectrum, and the valence band electrons is excited into the conduction band and excitation energy required is also reduced, which can cause a red shift phenomenon. When decreasing width of band gap, electrons is easy to transmit from valence band to conduct band, and the absorption capacity could be obviously enhanced in the lower energy areas, which should improve the catalytic properties and valuable instructional information to design a new generated sensor materials.

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**Reference**

Baraneedharan P., Hussain S., Imran, Dinesh V.P., et al., 2015, Lattice Doped Zn-$SnO_2$ Nanospheres: A systematic Exploration of Dopant Ion Effects on Structural, Optical, and Enhanced Gas Sensing Properties, Applied Surface Science, 357, 1511-1521, DOI: 10.1016/j.apsusc.2015.09.257.

Benedek R., Thackeray M.M., Yang L.H., 1999, Atomic Structure and Electrochemical Potential of $Li_1$+x$V_3O_8$, Physical Review B, 60(9), 6335, DOI: http://dx.doi.org/10.1103/PhysRevB.60.6335.

Borges P.D., Scolfaro L.M.R., Leite Alves H.W., Da Silva Jr. E.F., Assali L.V.C., 2012, Nanoscale Res. Lett., 7, 540, Doi: 10.1186/1556-276X-7-540

Chandran D., Nair L.S., Babu K.R., Deepa M., et al., 2015, Journal of Sol-gel Science and Technology, 76(3), 582-591, DOI: 10.1007/s10971-015-3808-z.

Dawar A.L., Jain A.K., Jagadish C., and Hartnagel H.L., 1995, Semiconducting Transparent Thin Films (Institute of Physics, London).

Dawar A.L., Joshi J.C., 1984, Semiconducting Transparent Thin Films: Their Properties and Applications, J. Mater. Sci., 19, 1-23, DOI: 10.1007/BF00552989.

Dean J.A. (ed.), 2008, Lange's Handbook of Chemistry, Fourteenthed, (McGraw-Hill, Inc., New York, 1992), 055502, DOI: 10.1103/PhysRevLett.101.055502.

Giuseppe G., Federico M., Adriano M., 2016, Constructal Design of the Mixing Zone Inside a Supersonic Ejector, International Journal of Heat and Technology, 34(S1), S109-S118, Dooi: 10.18280/ijht.34S114

Godinho K.G., Walsh A. and Watson G.W., 2009, Energetic and Electronic Structure Analysis of Intrinsic Defects in SnC >2, J. Phys. Chem. C., 113(1), 439-448, DOI: 10.1021/jp807753t.

Hammer B., Hansen L.B., Norskov J.K., 1999, Phys. Rev. B, 59, 7413-7421. DOI: Doi: 10.1103/PhysRevB.59.7413.

Hartnagel H.L., Dawa A.L., Jain A.K., et al., 1995, Semiconducting Transparent Thin Films (Institute of Physics, London).

Hays J., Punnoose A., Baldner R., Engelhard M.H., Peloquin J., Reddy K.M., 2005, Relationship between the Structural and Magnetic Properties of Co- doped $SnO_2$ Nanoparticles, Physical Review, 72(7), 075203, DOI: 10.1103/PhysRevB.72.075203.

Hohenberg P., Kohn W., 1964, Inhomogeneous Electron Gas, Phys. Rev., 136, B864-B871.

Janotti A., Walle C.G.V., 2011, LDA R U and Hybrid Functional Calculations for Defects in ZnO, $SnO_2$, and $TiO_2$, Phys. Status Solidi B 248, (4), 799–804, DOI 10.1002/pssb.201046384.

Kiliq C., Zunger A., 2002, Origins of Coexistence of Conductivity and Transparency in $SnO_2$, Phys. Phys. Rev. Lett., 88, 095501, DOI: 10.1103/PhysRevLett.88.095501.

Kim H., Gilmore C.M., Pique A., Horwitz J.S., 1999, Electrical, Ptical, and Structural Properties of Indium-tin-oxide Thin Films for Organic Light-emitting Devices, Journal of Applied Physics, 86(11), 6451-6461, DOI: 10.1063/1.371708.

Kim H.R., Haensch A., Kim I., Barsan N., Weimar U. and Lee J., 2011, Adv. Funct. Mater, 21(23), 4456-4463, DOI: 10.1002/adfm.201101154.

Lewis B.G., Paine D.C., 2000, Applications and Processing of Transparent Conducting Oxides, MRS Bull, 25(8), 22-27, DOI: 10.1557/mrs2000.147 (About DOI).

Li Y., Zhang Y.X., Kong X.R., et al., 2016, Investigation on Thermodynatic Performances of $Mg_2Sn$ Compound via First Principle Calculations, International Journal of Heat and Technology, 34(1), 110-114. Doi: 10.18280/ijht.340116.

Liu C.H., Zhang L., He Y., 1997, Properties and Mechanism Study of Ag Doped SnC>2 Thin Films as $H_2S$ Sensors, Thin Solid Films, 304, 13-15, DOI: 10.1016/S0040-6090(97)00107-7.

Liu Z.Y., Sun D.D., Guo P.and Leckie J. O., 2007, Nano Lett., 7(4), 1081-1085, DOI: 10.1021/nl061898e.

Look D.C., Claflin B., Ya. I. Alivov, et al., 2004, The Future of ZnO Light Emitters, Phys. Status Solidi A., 201, 2203–2212, DOI: 10.1002/pssa.200404803.

Monkhorst H.J. and Pack J.D., 1976, Special points for Brillouin-zone integrations, Phys. Rev. B: Condens. Matter Mater. Phys., 12, 5188, DOI: 10.1103/PhysRevB.13.5188.

Perdew J.P., Chevary J.A., Vosko S.H., 1993, Physical Review B, 46(11), 6671-6687, DOI: 10.1103/PhysRevB.46.6671.

Perdew J.P., Burke K., Ernzerhof M., 2006, Phys. Rev. Lett., 77, 3865−3868.

Qin G.Q., Li D.C., Feng Z.J., et al., 2009, First Principles Study on the Properties of P-type Conducting In: $SnO_2$, Thin Solid Films, 517(11), 3345-3349, DOI: 10.1016/j.tsf.2008.12.030.

Rajpure K.Y., Kusumade M.N., Neumann-Spallart M.N., et al., 2000, Effect of Sb Doping on Properties of Conductive Spray Deposited $SnO_2$ Thin Films, Materials Chemistry and Physics, 64(3), 184-188, DOI: 10.1016/S0254-0584(99)00256-4.

Ravindran P., Fast L., Korzhavyi P.A., Johansson B., Wills J., Eriksson O., 1998, J. Appl. Phys., 84 4891, DOI: 10.1063/1.368733.

Rossi F., et al., 2015, First-principles Non-equilibrium Dynamic Modelling of Agitated Thin-film Evaporators, CET, 43, 1429-1434, DOI: 10.3303/CET1543239.

Scanlon D.O., Watson G.W., 2012, On the possibility of p-type $SnO_2$, J. Mater. Chem., 22, 25236-25245, DOI: 10.1039/C2JM34352E.

Schleife A., Varley J.B., Fuchs F., Rodl C., Bechstedt F., Rinke P., A, 2013, Janotti and C. G. VandeWalle, Phys. Rev. B: Condens. Matter Mater. Phys., 87, 239901.

Snaith H.J., Ducat C., 2010, $SnO_2$-Based Dye-Sensitized Hybrid Solar Cells Exhibiting Near Unity Absorbed Photon-to-Electron Conversion Efficiency, Nano Lett., 10(4), 1259–1265, DOI: 10.1021/nl903809r.

Shieh S.R., Kubo A., Daffy T.S., Prakapenka V.B., Shen G.Y., 2006, High-pressure phases in $SnO_2$ to 117 GPa, Phys. Rev. B, 73, 014105, DOI: 10.1103/PhysRevB.73.014105.

Sigala C., Guyomard D., Verbaere A., et al., 1995, Solid State Ionics, 81(3), 167-170, DOI: 10.1016/0167-2738(95)00163-Z.

Singh A.K., Janotti A., Scheffler M., and Van de Walle C.G., 2008, Sources of Electrical Conductivity in $SnO_2$, Phys. Rev. Lett., DOI: 10.1103/PhysRevLett.101.055502.

Sun X.Q., Long R., Cheng X.F., et al., 2008, Structural, Electronic, and Optical Properties of N-doped $SnO_2$, Journal of Physical Chemistry, 112(26), 3345-3349, DOI: 10.1021/jp710564g.

Tang P., Holzwarth N., 2003, Electronic Structure of $FePO_4$, $LiFePO_4$, and Related Materials, Physical Review B, 68(16), 165107, DOI: 10.1103/PhysRevB.68.165107.

Triki A., Ezzeddine H.T., 2008, Numerical Simulation for One Dimensional Open Channel Transient Flow, International Journal of Heat and Technology, 26(1), 89-96.

Wang J.T., Yu W.L., Gao Y.L., 2015, First-principles Study on the Thermodynamic Defect and Crystal Structure of U-12.5 At% Nb Alloy, International Journal of Heat and Technology, 33(1), 175-180.

Yadav A.A., Pawar S.C., Patil D.H., et al., 2015, Journal of Alloys and Compounds, 652, 145-152, DOI: 10.1016/j.jallcom.2015.08.197.

Yang C.C., Chen M.S., Hong T.J., et al., 1995, Appl Phys Lett., 66, 2643, DOI: 10.1063/1.113111.

Yong L., Zhang Y.X., Tang J.Y., et al., 2015, First-principles Study on Lithium Intercalation of Silicon Anode Materials in Supercapacitor, Chemical Engineering Transactions, 46, 73-78, DOI: 10.3303/CET1546013.

Zhang S., Chen L.S., 2015, Semiconductor, Molecular Crystals and Oxide Temperature Pressure Phase Diagram, International Journal of Heat and Technology, 33(1), 123-128, DOI: 10.1002/adfm.200600431.