Novel Empirical Correlation Between the Optical Refractive Index and Energy Bandgap in Semiconductors: Comparative Study

Hosam Mohamed Gomaa (h_goumaa@yahoo.com)
Independent Researcher, https://orcid.org/0000-0002-4806-7867
I.S. Yahia
Ain Shams University Faculty of Education
H.Y. Zahran
Ain Shams University Faculty of Education

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Novel empirical correlation between the optical refractive index and energy bandgap in semiconductors: Comparative study

Hosam M. Gomaa[1*], I.S. Yahia[2,3], H.Y. Zahran[2,3,4]

[1]Independent Researcher, from Sakkara. Giza, Egypt.
[2]Advanced Functional Materials & Optoelectronic Laboratory (AFMOL), Department of Physics, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia.
[3]Research Center for Advanced Materials Science (RCAMS), King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia.
[4]Nanoscience Laboratory for Environmental and Biomedical Applications (NLEBA), Metallurgical Lab.1., Semiconductor Lab., Department of Physics, Faculty of Education, Ain Shams University, Roxy, 11757 Cairo, Egypt.

Abstract

This work is an attempt to review some of the most famous and important studies to correlate the optical-linear refractive index of a substance to its energy band-gap.The refractive index of different types of materials, like semiconductors, insulators, oxides, thin-films, and oxide glasses, has been reported in a large number of publications in attempts to the estimation of how it can be correlated to the optical band-gap. The present work can be considered as a comparative study between the most successful relations in correlating the refractive index to the energy gap. The careful reviewing of the previous studies to correlate the optical refractive index and energy gap led to concluded that Reddy and Ahmmed approximation was selected to develop a new realized form that can give a good fit to the experimental data and, hence, be used directly as an accurate formula in the theoretical studies. The obtained formula correlates the optical refractive index to the energy gap and the oxygen atom's electronegativity. Such relation has been used to calculate the refractive indices for more than 96 materials (elements/compounds) with a high agreement with the experimental data.

Keywords: Moss, Ravindra, Penn, energy gap, refractive index, electronegativity

*(Corresponding author: **Hosam M. Gomaa**)

E-mail: H_goumaa@yahoo.com

WhatsApp: +201001381061

1. Introduction

The Refractive index of the different categories of materials such as thin films, nanocomposites, nanopowder, chalcogenide glasses, oxide glasses, and all other semiconductors have been important to study because of their potential and advanced applications in the fields of electronic and Opto-electronic devices like the linear and non-linear optics, light-emitting diodes, photovoltaic cells, photo-detectors, lasers, modulators, Integrated circuits, and optical filtersThe optical refractive index is an important macroscopic parameter related to many microscopic properties of matter like; the internal local field and the matter's electronic polarizability. A refractive index is an important tool in many applications such as opto-electronic, linear, non-linear optics, optical switches, solar cell devices, photo-detectors, and lasers devices, Optical sensors, optical filters, and some integrated circuits [1-7]. Many researchers have attempted to propose, develop, and obtain simplified relations related to the optical refractive index to the energy gap [8-14]. Moss, Revindra et al., and Reddy et al. have proposed mathematical relations [15-18] that correlate the optical refractive index of the matter to its plasmon' energy gap, and they successfully used such relation to calculate some different parameters like bond length, bond energy, ….., etc. for the set of semiconductors. All these models showed an ability to calculate the optical refractive index with high accuracy but for a limited number of materials and limited energy ranges. Every day, there are many attempts to propose a new models or modify the oldest one to cover a large number of materials and long ranges of energy. Therefore, this study was performed to get more accurate and accurate comparisons between the optical refractive index and the energy gap, which may get the best fit for the experimental data. where the data of the refractive index and the bandgap were collected from many publications, for different materials. And then all data were simulated using each relation, separately, for comparison with the suggested relation, to Know-how if it has high accuracy in correlating the refractive index to the energy bandgap or not.

2. Simulation, Results and discussion

Moss has reported that the optical refractive index is a function of the absorption edge [19]; he stated that the optical refractive index and the edge of absorption are related by the following equation, where n is the optical refractive index, α is the absorption coefficient, and λ_e is the absorption edge wavelength:

$$n = 1 + \frac{1}{2\pi^2} \int \alpha \, d\lambda, \qquad \text{for} \quad f = 0 \tag{1}$$

$$n = 1 + \frac{1}{2\pi^2} \int \frac{\alpha}{1 - (\frac{\lambda}{\lambda_e})^2} \, d\lambda, \qquad \text{for} \quad f \neq 0 \tag{2}$$

$$n^4 \, E_g = 95, \tag{3}$$

Such relations tell that the average optical refractive index n equal to the area's value under the cure resulted from the plotting of the absorption coefficient α versus the wavelength λ regardless of the type of the absorption spectra. Moss' analysis [8, 20] showed the higher refractive indexes due to the high-intensity absorptions in the narrow bands, at wavelengths less than 1000 nm, which is too short concerning the absorption edge. Accordingly, Moss concluded that the optical refractive index in UV-region affects by the narrow absorption bands of semiconductors. Finally, Moss [21] stated that the relationships between the optical refractive index and energy gap could be described because of the dielectric theory energy levels, relation 3. This relation was used to calculate the refractive index corresponding to the energy gaps for different materials then compared with the measured values as seen in figure (1). This relation does not fit the experimental data at high energies > 3.35 eV. Also, the constant 95 does not refer to any physical meaning or quantity, which is considered a disadvantage in Moss' relation. Ravindra's relation is an empirical extension to what called Penn's model [8,22,23], where Ravindra et al. have said that the average energy gap (Penn gap) E_P differs from the optical band gap E_g by a constant value K [8,24], based on the fact that the valence and conduction bands in semiconductors are more or less parallel to each other, at least along with the symmetry directions. Gupta and Revindra used this concept in Penn's approximation, relation 5, to obtain a new relation, 6, correlate the optical refractive index to the energy gap; where ε_o, ω_p, E_g, and h are the static dielectric constant, plasma frequency, average energy gap, and Planck's constant, respectively. As seen in figure (2). It's clear that relation 6 does not fit the experimental data at high energies, above 3.35 eV, which consider a disadvantage point in Moss' relation as:

$$E_P = E_g + K, \tag{4}$$

$$\varepsilon_o = 1 + (\frac{h\omega_P}{2\pi E_g})^2, \tag{5}$$

$$n = K_1 + K_2 E_g + K_3 E_g^2 + K_4 E_g^3, \tag{6}$$

where (K_1 = 4.16 eV, K_2 = 1.12 eV^{-1}, K_3 = 0.31 eV^{-2}, and K_4 = 0.08 eV^{-3})

$$n = \sqrt{\frac{12.417}{E_g - 0.365}} \quad \textbf{(7)}$$

$$n = \left(1 + \frac{40.8}{E_g^2}\right)^{\frac{1}{4}}, \quad \textbf{(8)}$$

$$n = \sqrt{1 + \left(\frac{13.6}{E_g + 3.4}\right)^2}, \quad \textbf{(9)}$$

$$n = \sqrt{1 + \left(\frac{13.6}{3.72\,\Delta\chi + 3.4}\right)^2}, \quad \textbf{(10)}$$

$$n = 3.3668\, E_g^{-0.22234}, \quad \textbf{(11)}$$

$$n = \sqrt{\varepsilon}, \quad \textbf{(12)}$$

Reddy et al. have modified the original Moss' relation empirically to be as in relation 7, where they introduce the constant value 0.365, without giving any reason (why?). As seen in figure (3), relation 7 gives a bad fit to the experimental data in high energies and does not work well for low energy gap compounds. Relation 8 was proposed by Anani et al. [25,26] for the optical refractive index of some III-V semiconductors. Fig. (4) shows that Anani's relation can fit the experimental data well for the energies less than or equal to 0.62 eV only. Also, Harve et al. [6,26] have proposed a relation for the optical refractive index as a function of the energy gap, relation 9. As seen in figure (5), this relation gives a very good fit for the experimental data in medium and high energies. Duffy et al. [26,27] have correlated the optical refractive index to the energy gap by considering the electronegativity $\Delta\chi$ according to relation 10. As seen in Fig. (6), Duffy's relation has similar behavior to Harve's relation. As seen in Fig. (10), the value of the refractive index depends on the difference between the electronegativity of cations and the electronegativity of anions of the compound material $\Delta\chi = |\Delta\chi_{cation} - \Delta\chi_{anion}|$. This means that such relation is more applicable for the heterogeneous materials and does not suit mono-atomic, polyatomic, and homogeneous compound materials. Kumar and Singh [26] collected the experimental for both the optical refractive index and energy gap for different Martials from different sources. Then simulated the collected using computer software and obtain relation 11, where both contents 3.3668 and 0.32234 resulted have been obtained by optimizing the

experimental data of the optical refractive index and energy gap in the regression software. Relation 11 gives a good fit to the experimental data in low energies, but it's not valid at high energy values, as seen in Fig. (7). The present work proposes another empirical approximation that correlates the optical refractive index to the energy gap for different types of monoatomic, diatomic, and polyatomic materials. To get the aimed relation, authors have considered the relation of Reddy and Ahmmed approximation, relation 7, because it is a good modification for moss's model, which has the mathematical background. The authors compare Reddy and Ahmmed relation to the famous relation 12 [10], where ε is the static dielectric constant. Such comparison between relations 7 and 12 required that the quantities of Ander roots must be the same. Such comparison between relations 7 and 12 required that the quantities enclosed by roots must be the same. In other words, the quantity enclosed by the root of Reddy and Ahmed relation is a re-formalization for the dielectric constant. Accordingly, the authors state to develop Reddy and Ahmmed approximation to get simple empirical formula can be fit the experimental for different materials throughout arranging of energy extended from 0 eV to 11 eV. Authors focus on modifying the form of Reddy and Ahmmed relation by replacing the constants with another have physical meaning, such that the new form gives a good fit to the experimental data. . Authors focus on modifying the form of Reddy and Ahmmed relation by replacing the constants by another have physical meaning, such that the new form gives a good fit to the experimental data. The hard work led to getting in the following relation, 13;

$$n = \sqrt{\frac{A}{E_g^{0.5}} - B}, \qquad \textbf{(13)}$$

The constants A and B are the square and root square of the oxygen's Pauli-electronegativity (χ_O = 3.44). This formula was successfully used to calculate the refractive indices for more than 96 materials (elements/compounds). Tables. (1-3) exhibit the calculated refractive indices by the investigated formula and most famous related relations for comparison. All data were plotted as a function of the energy gap, as seen in Fig. (8); by looking to this Fig. (9) and inspecting all data in tables 1a, 1b, and 1c, it can see that the investigated formula has the best fitting to the experimental data in low and high energies.

3. Conclusion

$$n = \sqrt{\frac{A}{E_g^{0.5}} - B}$$

$$where\ A = 3.44^2\ \ and\ B = \sqrt{3.44}$$

The proposed formula is the best to correlate the optical refractive index of a material to its energy gap. Also, this formula is the best fit to the experimental data in low and high energy, the thing which nominates it to be a modification for all previous/other relations

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Table: (1a)

Samples	Energy, (eV)	n, (experimental)	n, (present study)	n, Ravinder	n, Moss	n, Harve	n, Reddy	n, Kumar
GeTe	0.1	6	5.964	4.0220	5.5518	3.9386	NA	7.0722
InSb	0.17	5.13	5.181	3.9786	4.8620	3.8678	NA	5.9604
InSb	0.18	3.95	5.103	3.9724	4.7931	3.8579	NA	5.8516
HgTe	0.2	3.74	4.960	3.9600	4.6685	3.8383	NA	5.6562
$CdSnAs_2$	0.26	3.7	4.621	3.9228	4.3721	3.7808	NA	5.1975
PbSe	0.28	4.59	4.529	3.9104	4.2918	3.7620	NA	5.0748
PbSe	0.29	4.79	4.485	3.9042	4.2543	3.7527	NA	5.0177
PbTe	0.31	5.35	4.404	3.8918	4.1840	3.7343	NA	4.9110
PbTe	0.32	5.73	4.366	3.8856	4.1509	3.7251	NA	4.8610
Te	0.33	5.3	4.330	3.8794	4.1191	3.7160	NA	4.8130
InAs	0.35	4.1	4.260	3.8670	4.0590	3.6980	NA	4.7226
InAS	0.36	3.5	4.227	3.8608	4.0305	3.6890	NA	4.6799
PbS	0.41	4.15	4.077	3.8298	3.9015	3.6450	7.6485	4.4878
S	0.47	2.04	3.925	3.7926	3.7706	3.5937	6.1885	4.2945
$CdGeAs_2$	0.61	3.4	3.646	3.7058	3.5326	3.4801	5.0071	3.9483
$ZnSnAs_2$	0.65	3.6	3.581	3.6810	3.4770	3.4491	4.8214	3.8683
Ge	0.66	4.05	3.565	3.6748	3.4637	3.4415	4.7800	3.8493
Ge	0.67	4	3.550	3.6686	3.4507	3.4339	4.7403	3.8307
GaSb	0.7	3.79	3.506	3.6500	3.4132	3.4113	4.6304	3.7770
GaSb	0.73	3.82	3.463	3.6314	3.3775	3.3890	4.5322	3.7263
$ZnGeAs_2$	0.85		3.314	3.5570	3.2514	3.3032	4.2213	3.5479
$CuAlTe_2$	0.9	3.3	3.259	3.5260	3.2053	3.2688	4.1190	3.4831
$CuInTe_2$	0.95	3.4	3.207	3.4950	3.1623	3.2353	4.0280	3.4229
$CuInSe_2$	0.96	2.9	3.197	3.4888	3.1540	3.2287	4.0110	3.4114
$CuGaTe_2$	1	3.3	3.159	3.4640	3.1220	3.2026	3.9463	3.3668
Si, $AgGaTe_2$	1.1	3.46	3.070	3.4020	3.0485	3.1395	3.8046	3.2649
Si	1.12	3.47	3.054	3.3896	3.0348	3.1272	3.7791	3.2460
$CdSnP_2$	1.17	3.1	3.014	3.3586	3.0018	3.0969	3.7190	3.2007
AS	1.2	3.35	2.991	3.3400	2.9829	3.0791	3.6852	3.1746
InP	1.35	3.1	2.886	3.2470	2.8963	2.9935	3.5361	3.0564
GaAs	1.42	4.02	2.842	3.2036	2.8600	2.9555	3.4759	3.0070
GaAs	1.43	3.3	2.836	3.1974	2.8549	2.9502	3.4677	3.0002

Table: (1b)

Samples	Energy, (eV)	n, (experimental)	n, (present study)	n, Ravinder [ ]	n, Moss [ ]	n, Harve [ ]	n, Reddy [ ]	n, Kumar [ ]
$CuInS_2$	1.5	2.6	2.794	3.1540	2.8210	2.9134	3.4130	2.9543
$CdSiAs_2$	1.55	3.5	2.766	3.1230	2.7980	2.8878	3.3764	2.9232
CdTe	1.56	2.82	2.760	3.1168	2.7935	2.8828	3.3693	2.9172
CdTe	1.58	2.7	2.749	3.1044	2.7846	2.8727	3.3553	2.9052
AlSb	1.6	3.19	2.739	3.0920	2.7759	2.8628	3.3417	2.8935
$ZnSnP_2$	1.62	2.9	2.728	3.0796	2.7673	2.8529	3.3283	2.8819
$CuGaSe_2$, $ZnSiAs_2$	1.7	2.8	2.687	3.0300	2.7341	2.8142	3.2773	2.8375
$CdGeP_2$	1.72	3.3	2.677	3.0176	2.7261	2.8047	3.2651	2.8268
CdSe	1.74	2.49	2.668	3.0052	2.7183	2.7954	3.2532	2.8163
$AgGaSe_2$	1.8	2.8	2.639	2.9680	2.6953	2.7676	3.2186	2.7857
$AgInS_2$	1.86	2.5	2.612	2.9308	2.6733	2.7406	3.1858	2.7564
$ZnGeP_2$	1.99	3.1	2.556	2.8502	2.6286	2.6841	3.1201	2.6970
$ZnSiP_2$	2.1	3.1	2.512	2.7820	2.5934	2.6385	3.0694	2.6507
AlAs	2.15	2.87	2.493	2.7510	2.5782	2.6184	3.0477	2.6306
AlAs	2.18	3	2.482	2.7324	2.5693	2.6065	3.0350	2.6189
$CdSiP_2$	2.2	3.1	2.475	2.7200	2.5635	2.5987	3.0267	2.6112
AlSb	2.22	3.19	2.467	2.7076	2.5577	2.5909	3.0185	2.6036
GaP	2.24	2.9	2.460	2.6952	2.5519	2.5832	3.0104	2.5961
ZnTe, SeN	2.26	2.7	2.453	2.6828	2.5463	2.5755	3.0025	2.5887
Se, ZnTe	2.3	2.45	2.439	2.6580	2.5351	2.5604	2.9868	2.5741
CdS, $CuGaS_2$	2.4	2.38	2.405	2.5960	2.5083	2.5235	2.9494	2.5390
AIP	2.45	2.75	2.389	2.5650	2.4954	2.5055	2.9316	2.5222
cdO	2.5	2.32	2.373	2.5340	2.4828	2.4879	2.9143	2.5058
ZnSe	2.58	2.43	2.348	2.4844	2.4633	2.4603	2.8876	2.4805
SiC	2.6	2.6	2.342	2.4720	2.4586	2.4536	2.8811	2.4743
$CuAlSe_2$, $AgGaS_2$	2.7	2.6	2.312	2.4100	2.4355	2.4204	2.8498	2.4444
GaP	2.78	3.35	2.290	2.3604	2.4178	2.3948	2.8259	2.4215
CuBr	3	2.12	2.231	2.2240	2.3722	2.3278	2.7649	2.3628
SiC	3.1		2.206	2.1620	2.3528	2.2989	2.7393	2.3379
GaN	3.25	2.4	2.170	2.0690	2.3252	2.2574	2.7030	2.3026
CuCl	3.31	2.19	2.156	2.0318	2.3146	2.2413	2.6891	2.2891

Table: (1c)

Samples	Energy, (eV)	n, (experimental)	n, (present study)	n, Ravinder [ ]	n, Moss [ ]	n, Harve [ ]	n, Reddy [ ]	n, Kumar [ ]
CuCl	3.33	1.97	2.152	2.0194	2.3111	2.2361	2.6846	2.2846
ZnO	3.35	2.01	2.147	2.0070	2.3076	2.2308	2.6801	2.2802
$CuAlS_2$	3.5	2.4	2.114	1.9140	2.2825	2.1925	2.6474	2.2482
ZnS	3.54	2.27	2.106	1.8892	2.2760	2.1826	2.6390	2.2400
ZnS	3.68	2.35	2.077	1.8024	2.2541	2.1489	2.6107	2.2122
ZnO	3.7	1.92	2.073	1.7900	2.2510	2.1443	2.6068	2.2083
AIN	3.8	2.16	2.053	1.7280	2.2361	2.1212	2.5876	2.1894
S	3.82	2.04	2.049	1.7156	2.2331	2.1167	2.5839	2.1857
BN	4.6	2.1	1.914	1.2320	2.1318	1.9596	2.4557	2.0587
C	5.4	2.35	1.799	0.7360	2.0480	1.8305	2.3517	1.9550
GeO_2	5.6	1.6	1.774	0.6120	2.0295	1.8023	2.3289	1.9322
RbI	5.8	1.64	1.749	0.4880	2.0117	1.7755	2.3072	1.9104
NaI	5.9	1.77	1.737	0.4260	2.0032	1.7626	2.2967	1.8999
KI	6.17	1.67	1.706	0.2586	1.9809	1.7293	2.2695	1.8727
CsI	6.2	1.78	1.702	0.2400	1.9785	1.7257	2.2666	1.8698
CsI	6.3	1.82	1.691	0.1780	1.9706	1.7140	2.2570	1.8602
CsBr	6.9	1.69	1.628	NA	1.9263	1.6492	2.2033	1.8064
CsBr	7	1.67	1.618	NA	1.9194	1.6393	2.1949	1.7981
RbBr	7.2	1.55	1.598	NA	1.9059	1.6201	2.1787	1.7818
NaBr	7.3	1.64	1.589	NA	1.8993	1.6108	2.1708	1.7739
CsCl	7.4	1.64	1.580	NA	1.8929	1.6017	2.1630	1.7662
NaBr	7.5	1.64	1.570	NA	1.8865	1.5928	2.1554	1.7585
KBr	7.6	1.55	1.561	NA	1.8803	1.5841	2.1479	1.7510
CsCl	8	1.61	1.526	NA	1.8563	1.5511	2.1192	1.7223
RbCl	8.3	1.49	1.501	NA	1.8393	1.5281	2.0989	1.7020
SiO2	8.4	1.56	1.493	NA	1.8338	1.5208	2.0923	1.6955
KCl	8.5	1.49	1.485	NA	1.8284	1.5136	2.0859	1.6890
NaCl	8.9	1.54	1.453	NA	1.8075	1.4862	2.0610	1.6641
NiF2	9	1.56	1.446	NA	1.8025	1.4797	2.0550	1.6582
CsF	10	1.48	1.374	NA	1.7556	1.4211	1.9995	1.6028
KF	10.33	1.36	1.352	NA	1.7414	1.4040	1.9827	1.5861
RbF	10.4	1.4	1.347	NA	1.7385	1.4005	1.9793	1.5827
NaF	10.41	1.33	1.346	NA	1.7381	1.4000	1.9788	1.5822

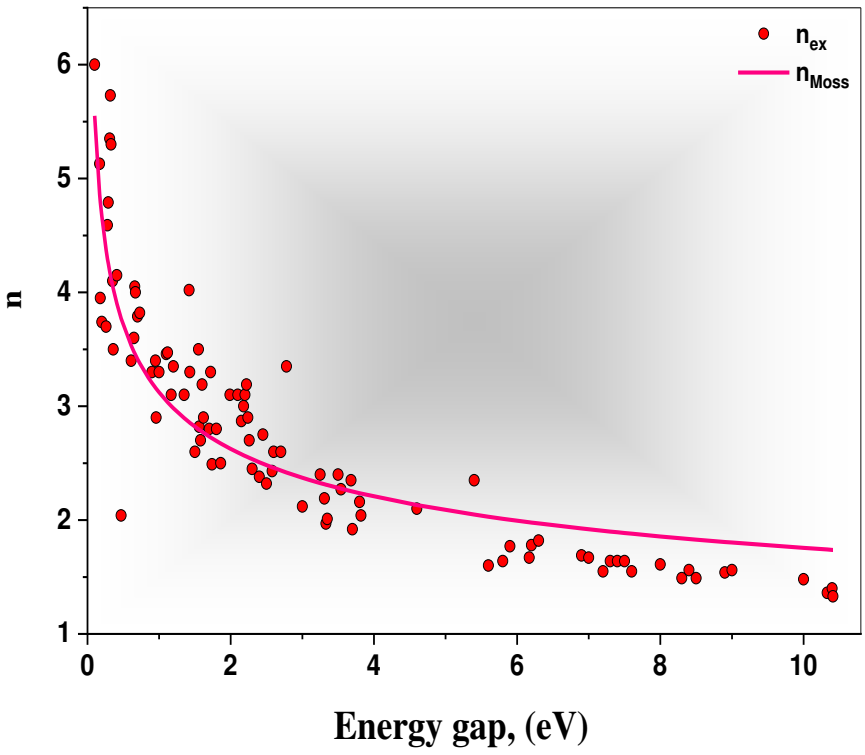

Fig. (1): Moss's relation: $n^4 E_g = 95$,

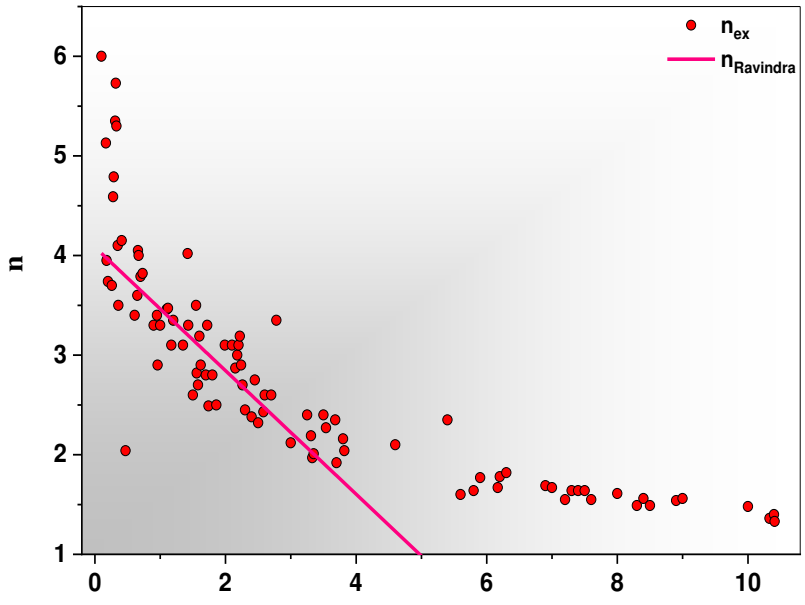

Fig. (2): Ravindra relation: $n = 4.084 - 0.62 E_g$

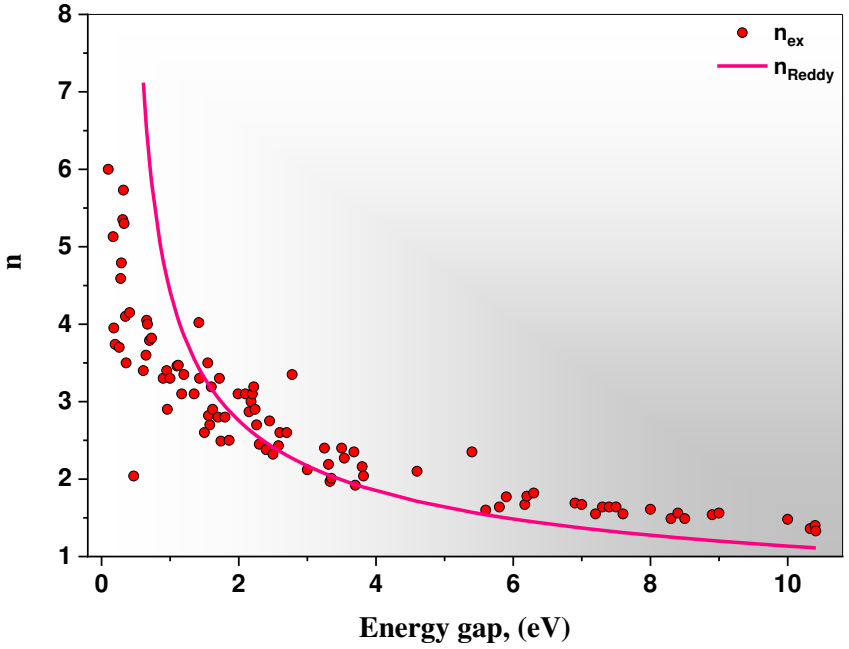

Fig. (3): Reddy relation: $n = \sqrt{\frac{12.417}{E_g - 0.365}}$

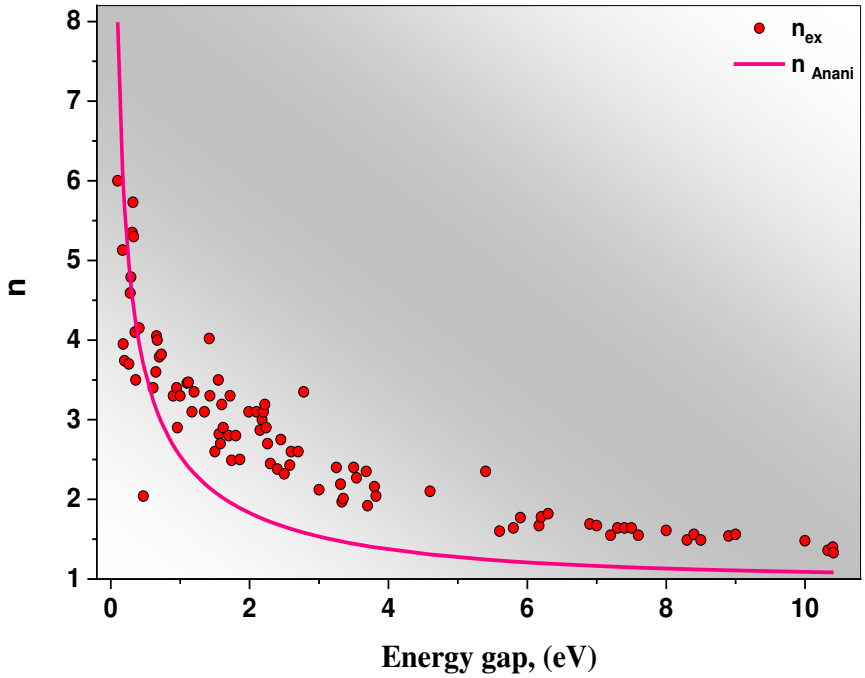

Fig. (4): Anani relation: $n = (1 + \frac{40.8}{E_g^2})^{\frac{1}{4}}$

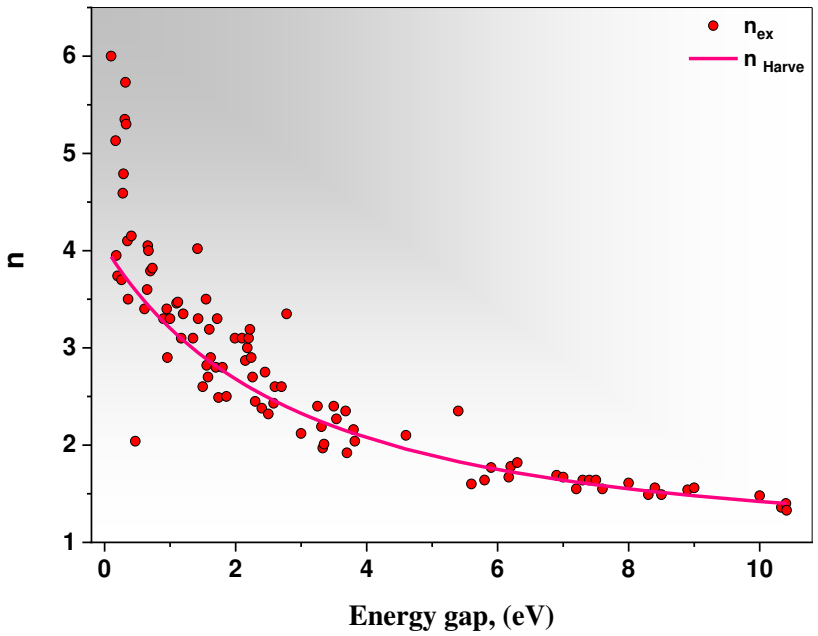

Fig. (5): Harve relation: $n = \sqrt{1 + (\frac{13.6}{E_g+3.4})^2}$

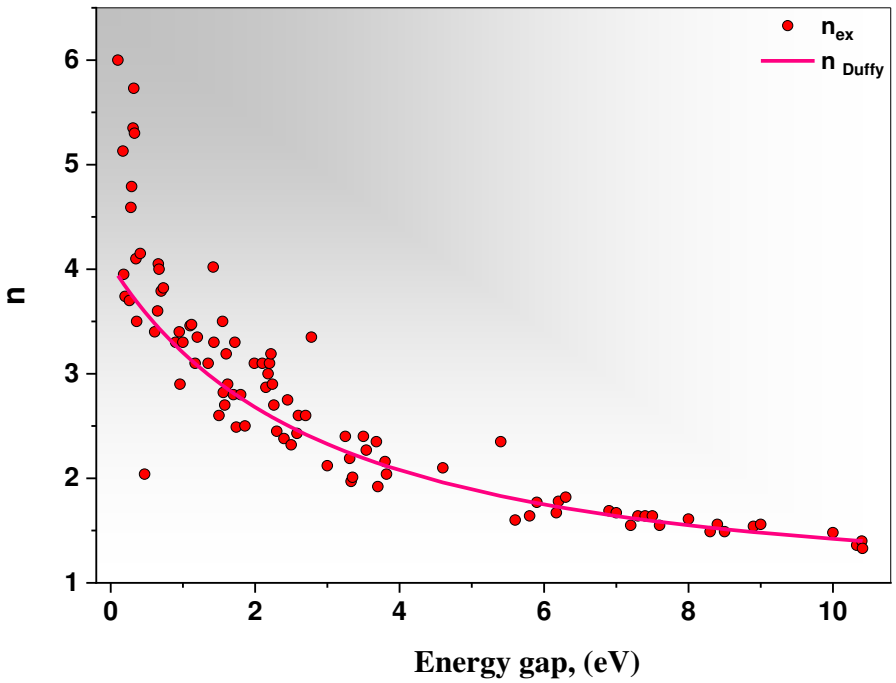

Fig. (6): Duffy relation: $n = \sqrt{1 + (\frac{13.6}{3.72\,\Delta\chi+3.4})^2}$, $\Delta\chi = 0.2688E_g$

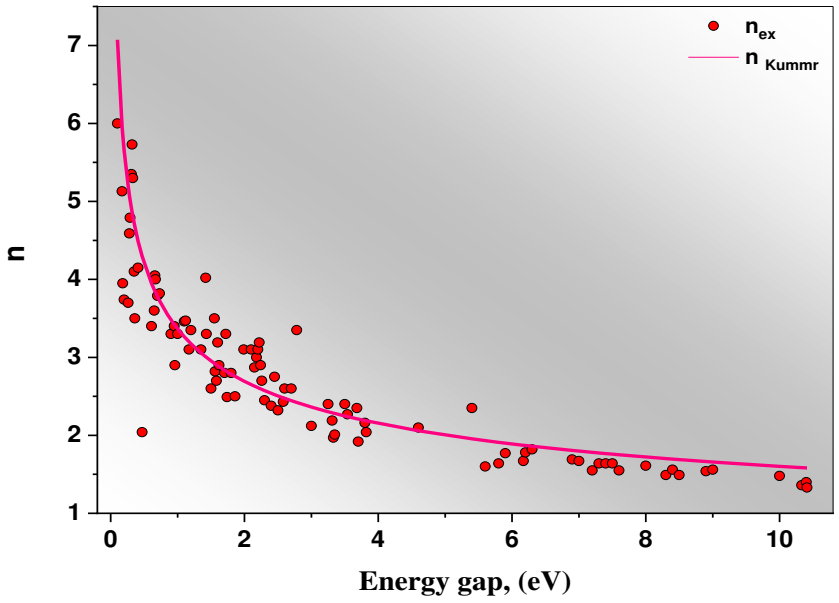

Fig. (7):: Kumar relation: $n = 3.3668\ E_g^{-0.22234}$

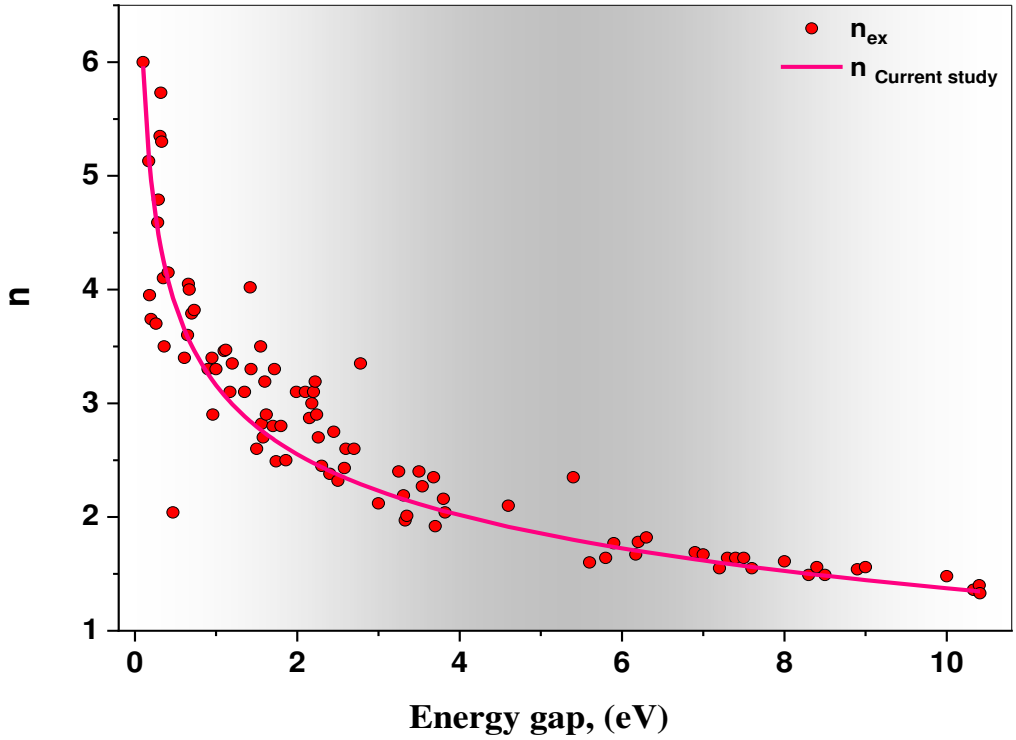

Fig. (8): Current study $n = \sqrt{\frac{A}{E_g^{0.5}} - B}$, *where* $A = 3.44^2$ *and* $B = \sqrt{3.44}$

Figures

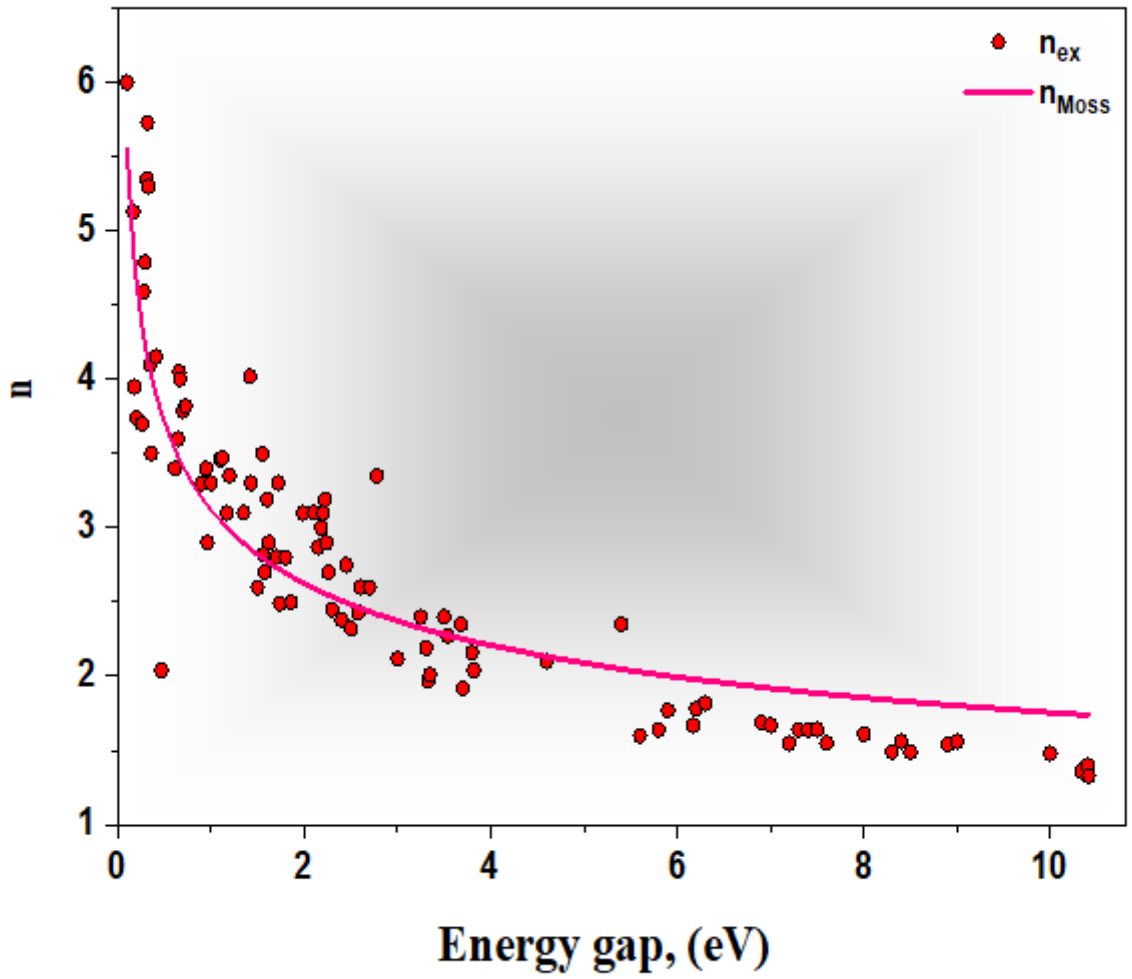

Figure 1

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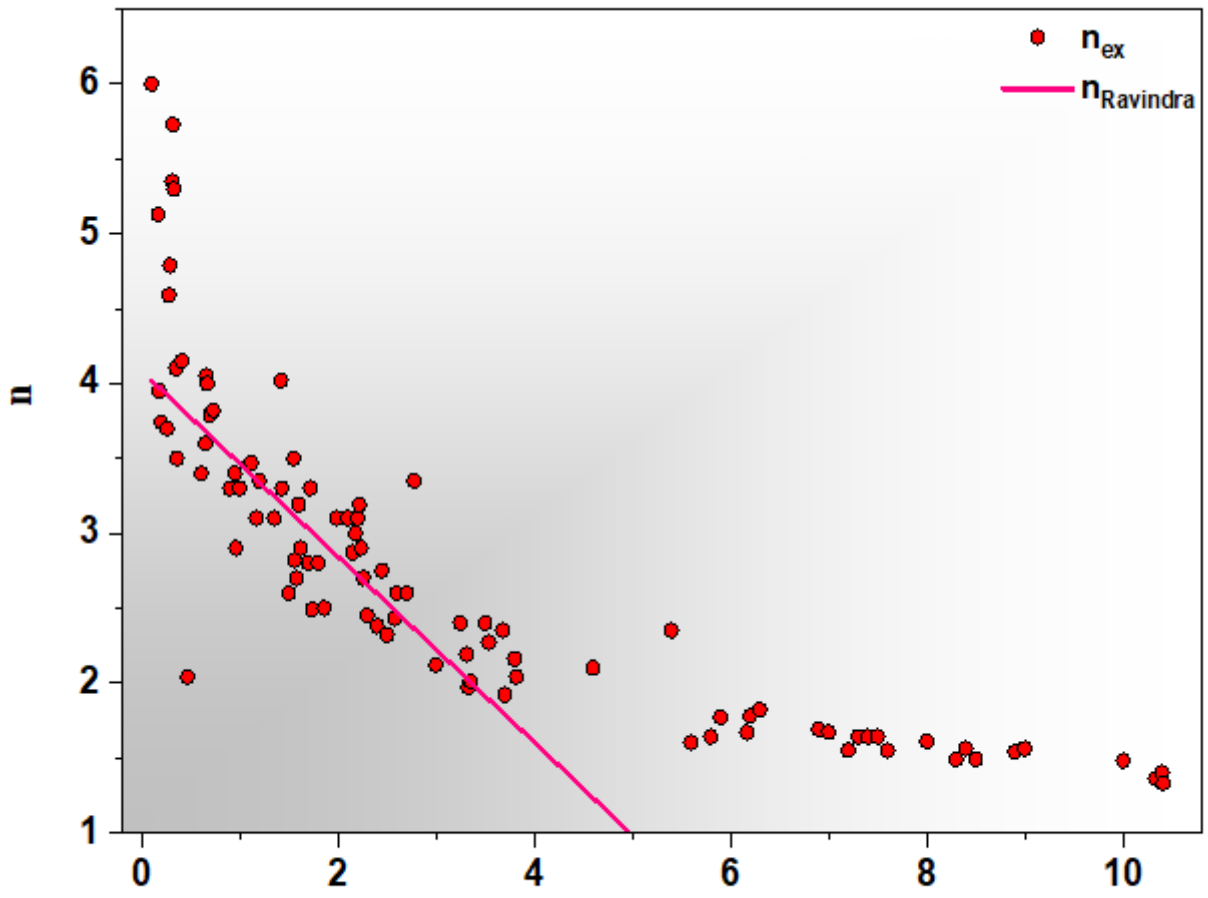

Figure 2

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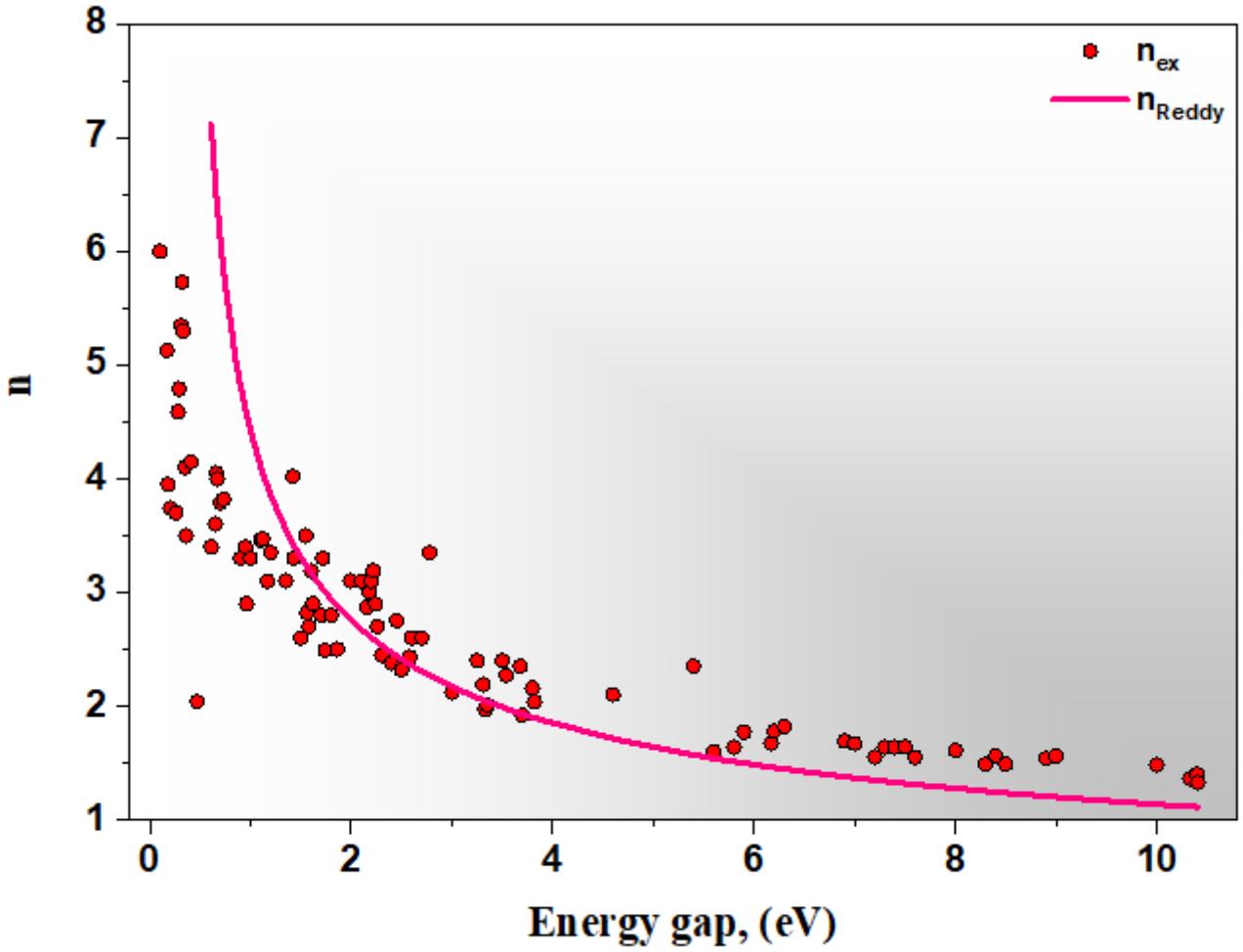

Figure 3

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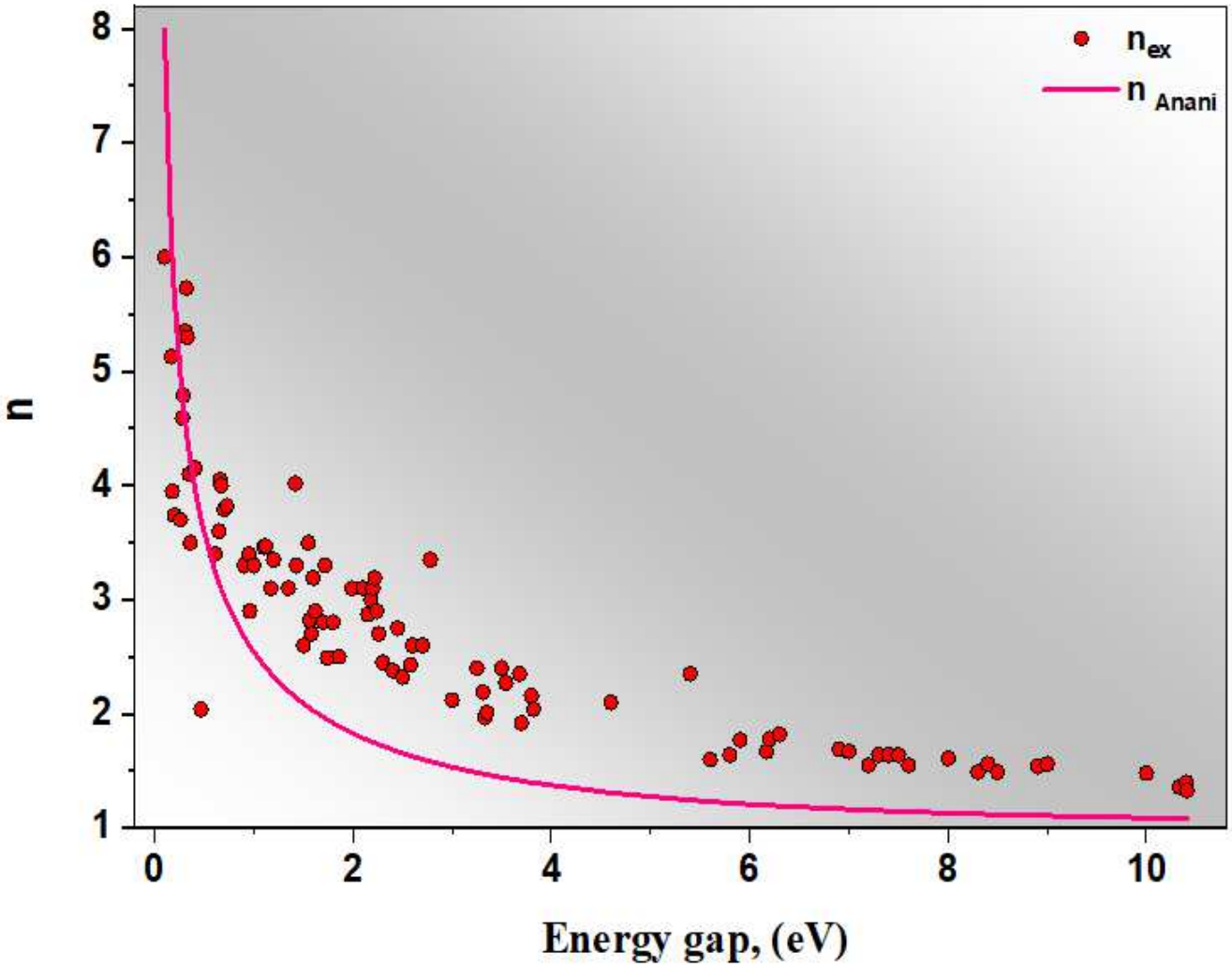

Figure 4

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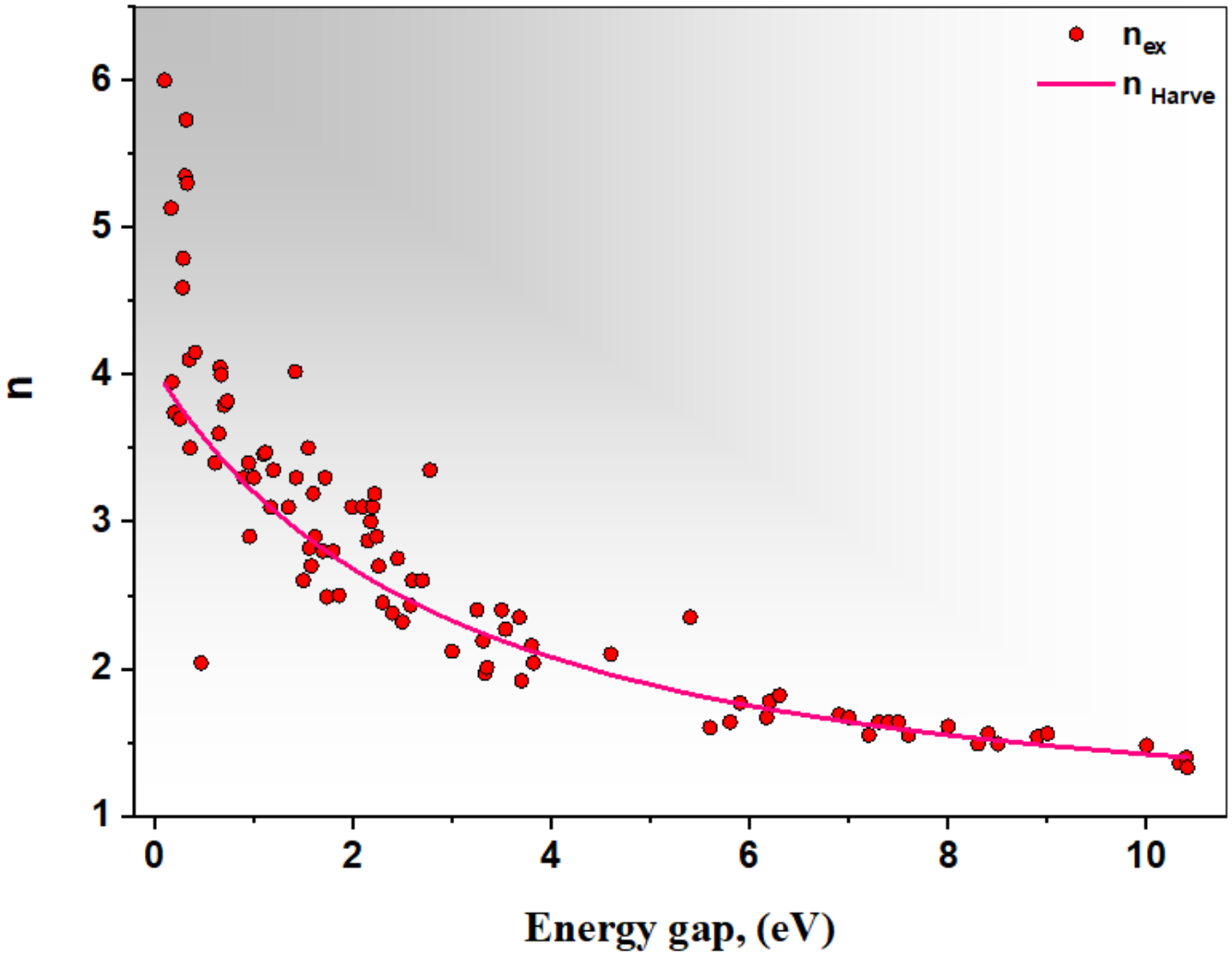

Figure 5

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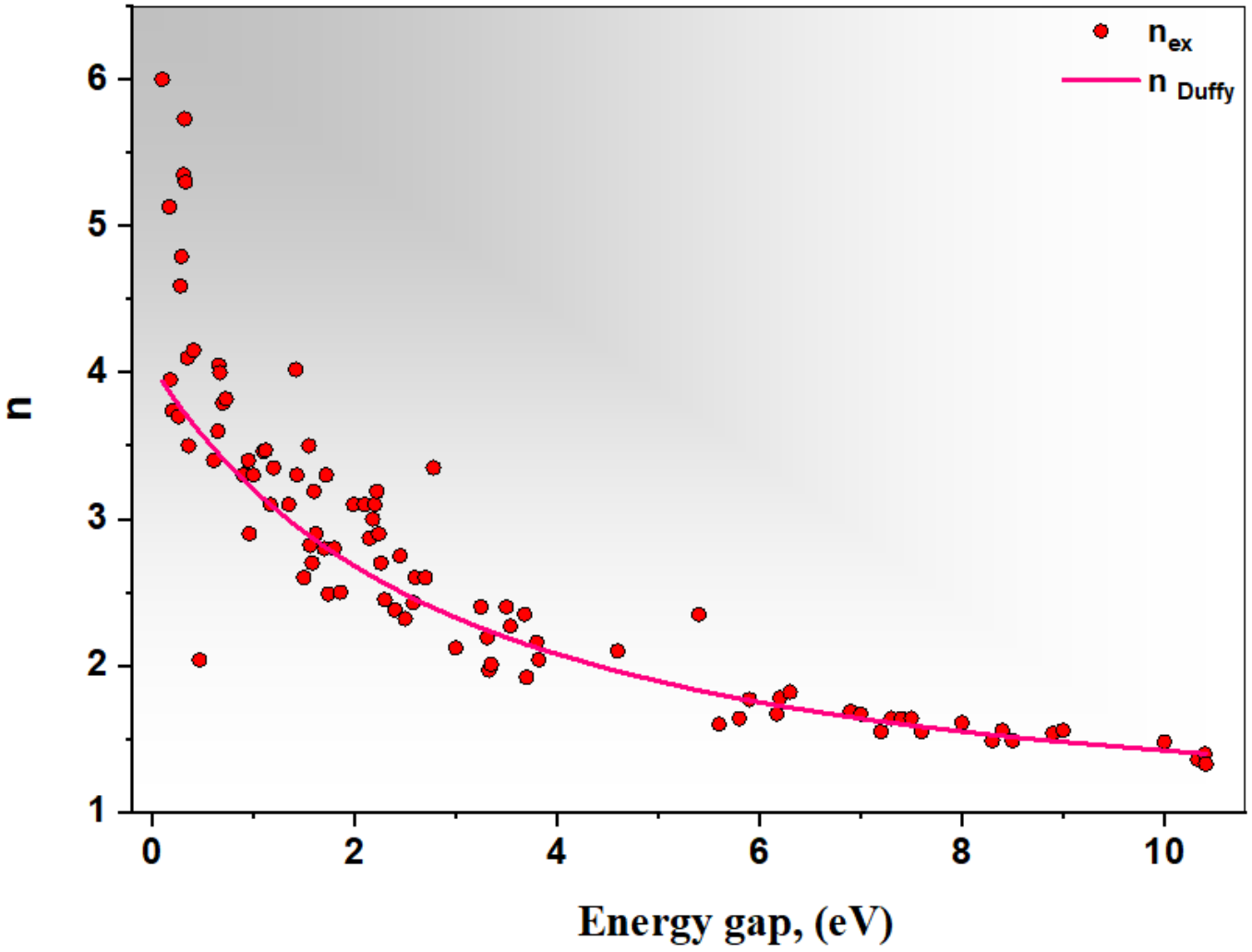

Figure 6

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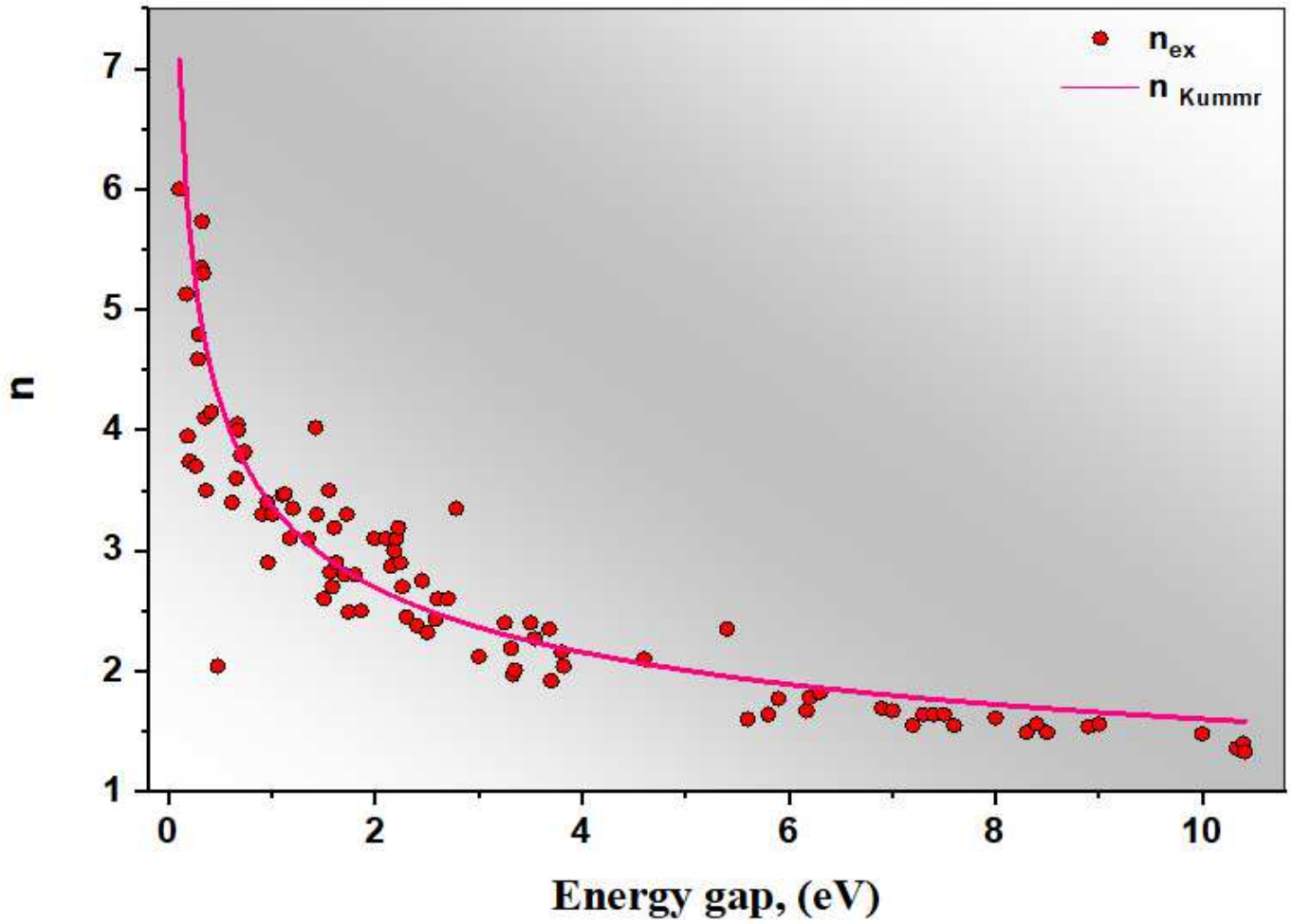

Figure 7

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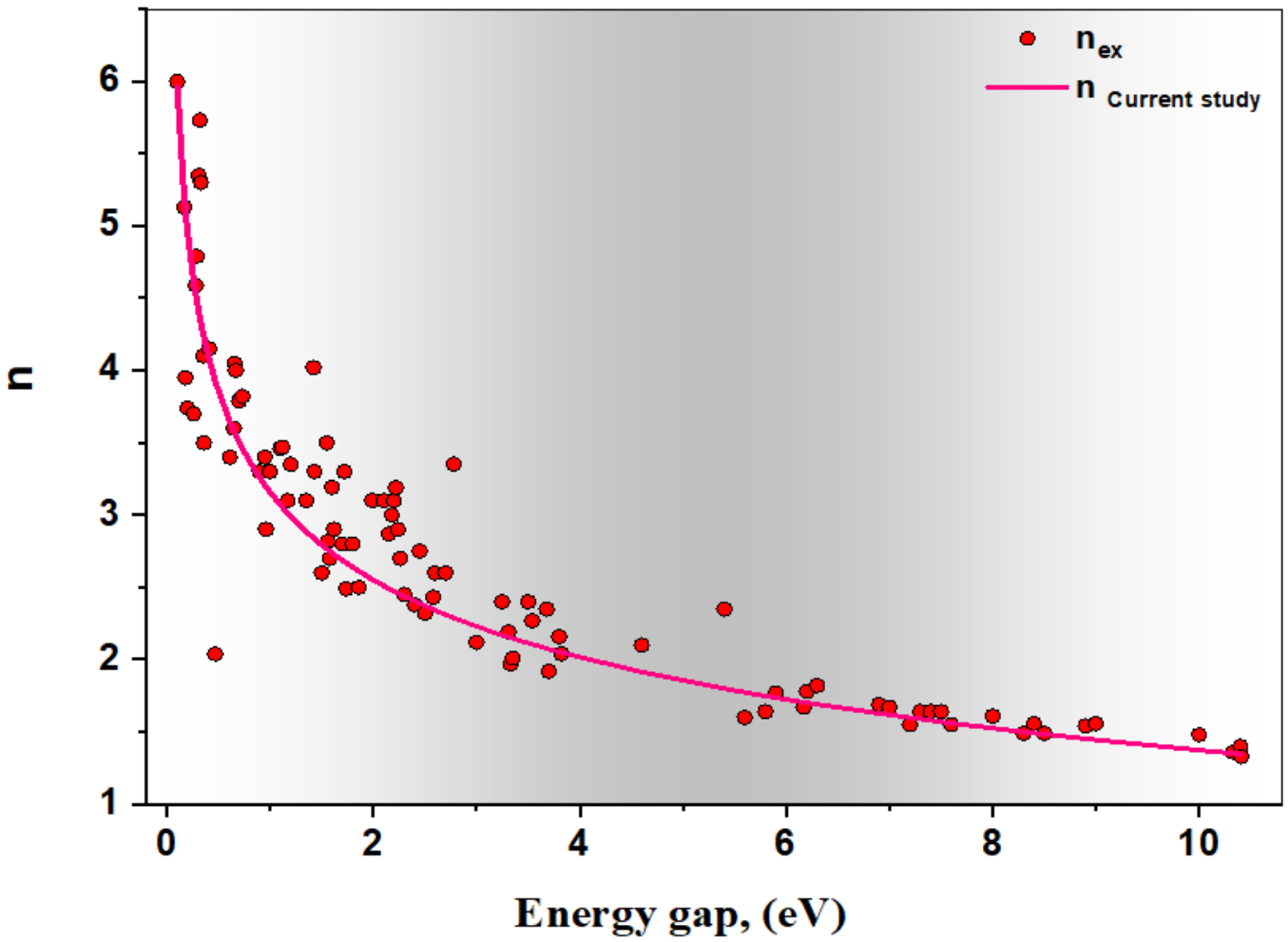

Figure 8

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