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Research Areas

Materials Science, Condensed Matter 1: Structural, Mechanical and Thermal Properties, Intensive Article 2: Electronic Structure, Electric, Magnetic and Optical Properties

Academic Titles / Tasks

Associate Professor, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Physics, 2016 - Continues

Advising Theses

Sürücü G., A density functional theory investigation for solid state hydrogen storage materials, Doctorate, A.Gencer(Student), 2019

Sürücü G., The effect of hydrogen on the mechanical and vibrational properties of $\text{LaMgNi}_4\text{H}_x$ ($x=1, 4, 7$), Post Graduate, M.BAHADIR(Student), 2016

Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

- I. **Electronic, optical and thermodynamic characteristics of $\text{Bi}_{12}\text{SiO}_{20}$ sillenite: First principle calculations**
Isik M., SÜRÜCÜ G., Gencer A., HASANLI N.
Materials Chemistry and Physics, vol.267, 2021 (Journal Indexed in SCI Expanded)
- II. **Enhanced hydrogen storage of a functional material: Hf_2CF_2 MXene with Li decoration**
Gencer A., AYDIN S., Surucu O., Wang X., Deligoz E., SÜRÜCÜ G.
Applied Surface Science, vol.551, 2021 (Journal Indexed in SCI Expanded)
- III. **First principles study of $\text{Bi}_{12}\text{GeO}_{20}$: Electronic, optical and thermodynamic characterizations**
Isik M., Sürücü G., Gencer A., Hasanlı N.
Materials Today Communications, vol.27, 2021 (Journal Indexed in SCI Expanded)
- IV. **Electronic and thermodynamic properties of lanthanum tetraboride on low-temperature experimental and ab-initio calculation data**
Sürücü G., Ozısık H., Deligoz E., Shein I., Matovnikov A., Mitroshenkov N., Morozov A., Novikov V.
Journal of Alloys and Compounds, vol.862, 2021 (Journal Indexed in SCI Expanded)
- V. **The investigation of electronic nature and mechanical properties under spin effects for new half-metallic ferromagnetic chalcogenides Ag_3CrX_4 ($X = \text{S, Se, and Te}$)**
Erkisi A., YILDIZ B., Wang X., Isik M., Ozcan Y., SÜRÜCÜ G.
Journal of Magnetism and Magnetic Materials, vol.519, 2021 (Journal Indexed in SCI Expanded)

- VI. **Editorial: Computational Modeling of Spintronic Materials**
Wang X., Cheng Z., Surucu G.
Frontiers in Materials, vol.7, 2021 (Journal Indexed in SCI Expanded)
- VII. **The investigation of electronic, anisotropic elastic and lattice dynamical properties of MAB phase nanolaminated ternary borides: M_2AlB_2 ($M = Mn, Fe$ and Co) under spin effects**
Surucu G., YILDIZ B., Erkisi A., Wang X., Surucu O.
JOURNAL OF ALLOYS AND COMPOUNDS, vol.838, 2020 (Journal Indexed in SCI)
- VIII. **First-principles studies of $Tin+1SiN(n)$ ($n=1, 2, 3$) MAX phase**
Surucu G., Gullu H. H., CANDAN A., YILDIZ B., Erkisi A.
PHILOSOPHICAL MAGAZINE, vol.100, no.17, pp.2183-2204, 2020 (Journal Indexed in SCI)
- IX. **Anisotropic mechanical properties of $Tl_4Ag_{18}Te_{11}$ compound with low thermal conductivity**
Gencer A., Surucu O., Surucu G., DELİGÖZ E.
JOURNAL OF SOLID STATE CHEMISTRY, vol.289, 2020 (Journal Indexed in SCI)
- X. **$Pnma$ metal hydride system $LiBH$: a superior topological semimetal with the coexistence of twofold and quadruple degenerate topological nodal lines**
Zhou F., Ding G., Cheng Z., Surucu G., Chen H., Wang X.
JOURNAL OF PHYSICS-CONDENSED MATTER, vol.32, no.36, 2020 (Journal Indexed in SCI)
- XI. **Investigation of structural, electronic, magnetic and lattice dynamical properties for $XCoBi$ ($X: Ti, Zr, Hf$) Half-Heusler compounds**
Surucu G., IŞIK M., CANDAN A., Wang X., Gullu H. H.
PHYSICA B-CONDENSED MATTER, vol.587, 2020 (Journal Indexed in SCI)
- XII. **Rich topological nodal line bulk states together with drum-head-like surface states in $NaAlGe$ with anti- $PbFCl$ type structure**
Wang X., Ding G., Cheng Z., Surucu G., Wang X., Yang T.
JOURNAL OF ADVANCED RESEARCH, vol.23, pp.95-100, 2020 (Journal Indexed in SCI)
- XIII. **Coexistence of parabolic and linear band crossings and electron-doped spin-gapless properties in rhombohedral type YbB_3**
Yang T., Cheng Z., Surucu G., Wang X.
JOURNAL OF ALLOYS AND COMPOUNDS, vol.823, 2020 (Journal Indexed in SCI)
- XIV. **Lattice dynamical and thermo-elastic properties of M_2AlB ($M = V, Nb, Ta$) MAX phase borides**
Surucu G., Gencer A., Wang X., Surucu O.
JOURNAL OF ALLOYS AND COMPOUNDS, vol.819, 2020 (Journal Indexed in SCI)
- XV. **$CaXH_3$ ($X = Mn, Fe, Co$) perovskite-type hydrides for hydrogen storage applications**
SÜRÜCÜ G., Gencer A., Candan A., Gullu H. H., IŞIK M.
INTERNATIONAL JOURNAL OF ENERGY RESEARCH, vol.44, no.3, pp.2345-2354, 2020 (Journal Indexed in SCI)
- XVI. **Novel topological nodal lines and exotic drum-head-like surface states in synthesized $CsCl$ -type binary alloy $TiOs$**
Wang X., Ding G., Cheng Z., Surucu G., Wang X., Yang T.
JOURNAL OF ADVANCED RESEARCH, vol.22, pp.137-144, 2020 (Journal Indexed in SCI)
- XVII. **Properties of $BaYO_3$ perovskite and hydrogen storage properties of $BaYO_{3Hx}$**
GENCER A., Surucu G.
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.45, no.17, pp.10507-10515, 2020 (Journal Indexed in SCI)
- XVIII. **Enhancement of hydrogen storage properties of Ca_3CH antiperovskite compound with hydrogen doping**
GENCER A., Surucu G.
INTERNATIONAL JOURNAL OF ENERGY RESEARCH, vol.44, no.1, pp.567-573, 2020 (Journal Indexed in SCI)
- XIX. **Electronic, mechanical and lattice dynamical properties of YXB_4 ($X = Cr, Mn, Fe, and Co$) compounds**
CANDAN A., SÜRÜCÜ G., Gencer A.
PHYSICA SCRIPTA, vol.94, no.12, 2019 (Journal Indexed in SCI)
- XX. **Density functional theory (DFT) study of $BaScO_{3H0.5}$ compound and its hydrogen storage properties**

- GENCER A., Surucu G.
CANADIAN JOURNAL OF PHYSICS, vol.97, no.11, pp.1191-1199, 2019 (Journal Indexed in SCI)
- XXI. **Transition metal-doped janus monolayer SMOSe with excellent thermal spin filter and spin Seebeck effect**
Ding G., Wei M., Surucu G., Liang Z., Wang X.
APPLIED SURFACE SCIENCE, vol.491, pp.750-756, 2019 (Journal Indexed in SCI)
- XXII. **First principles study on the structural, electronic, mechanical and lattice dynamical properties of XRhSb (X = Ti and Zr) paramagnet half-Heusler antimonides**
SÜRÜCÜ G., CANDAN A., Erkisi A., Gencer A., Gullu H. H.
Materials Research Express, vol.6, no.10, 2019 (Journal Indexed in SCI Expanded)
- XXIII. **First principles study on new half-metallic ferromagnetic ternary zinc-based sulfide and telluride (Zn₃VS₄ and Zn₃VTe₄)**
Erkisi A., YILDIZ B., DEMİR K., SÜRÜCÜ G.
MATERIALS RESEARCH EXPRESS, vol.6, no.7, 2019 (Journal Indexed in SCI)
- XXIV. **Investigation of structural, electronic and lattice dynamical properties of XNiH₃ (X = Li, Na and K) perovskite type hydrides and their hydrogen storage applications**
GENCER A., Surucu G.
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.44, no.29, pp.15173-15182, 2019 (Journal Indexed in SCI)
- XXV. **MgTiO₃H_x and CaTiO₃H_x perovskite compounds for hydrogen storage applications**
GENCER A., Surucu G., AL S.
International Journal of Hydrogen Energy, vol.44, no.23, pp.11930-11938, 2019 (Journal Indexed in SCI Expanded)
- XXVI. **The electronic and elasticity properties of new half-metallic chalcogenides Cu(3)TMCh(4) (TM = Cr, Fe and Ch = S, Se, Te): an ab initio study**
ERKİŞİ A., SÜRÜCÜ G.
PHILOSOPHICAL MAGAZINE, vol.99, no.4, pp.513-529, 2019 (Journal Indexed in SCI)
- XXVII. **The effect of hydrogen on the electronic, mechanical and phonon properties of LaMgNi₄ and its hydrides for hydrogen storage applications**
Baysal M. B. , SÜRÜCÜ G., DELİGÖZ E., ÖZİŞİK H.
International Journal of Hydrogen Energy, vol.43, no.52, pp.23397-23408, 2018 (Journal Indexed in SCI Expanded)
- XXVIII. **Electronic and lattice dynamical properties of Ti₂SiB MAX phase**
Gencer A., SÜRÜCÜ G.
MATERIALS RESEARCH EXPRESS, vol.5, no.7, 2018 (Journal Indexed in SCI)
- XXIX. **The structural, electronic, magnetic, and mechanical properties of perovskite oxides PbM_{1/2}Nb_{1/2}O₃ (M = Fe, Co and Ni)**
ERKİŞİ A., SÜRÜCÜ G., DELİGÖZ E.
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.32, no.6, 2018 (Journal Indexed in SCI)
- XXX. **Investigation of structural, electronic, anisotropic elastic, and lattice dynamical properties of MAX phases borides: An Ab-initio study on hypothetical &ITM(2)AB&IT (M = &ITTi&IT, &ITZr&IT, & A = &ITAl&IT, &ITGa&IT, &ITIn&IT) compounds**
Sürücü G.
MATERIALS CHEMISTRY AND PHYSICS, vol.203, pp.106-117, 2018 (Journal Indexed in SCI)
- XXXI. **DFT-based ab-initio study of half-Heusler KCaP compound**
Mogulkoc Y., ÇİFTÇİ Y., SÜRÜCÜ G.
JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS, vol.20, pp.61-68, 2018 (Journal Indexed in SCI)
- XXXII. **The Investigation of Electronic, Elastic and Vibrational Properties of an Interlanthanide Perovskite: PrYbO₃**
KADEROĞLU Ç., SÜRÜCÜ G., ERKİŞİ A.
JOURNAL OF ELECTRONIC MATERIALS, vol.46, no.10, pp.5827-5836, 2017 (Journal Indexed in SCI)
- XXXIII. **An ab initio study on the investigation of structural, electronic, mechanical and lattice dynamical**

properties of the M₂AX type MAX phases Sc₂AlB_{0.5}Co_{0.5}, Sc₂AlB_{0.5}N_{0.5} and Sc₂AlCo_{0.5}N_{0.5} compounds

SÜRÜCÜ G., SÜRÜCÜ G.

Materials Research Express, vol.4, no.10, 2017 (Journal Indexed in SCI Expanded)

- XXXIV. **The investigation of electronic, mechanical and lattice dynamical properties of PdCoX (X = Si and Ge) half-Heusler metallics in α , β and γ structural phases: an ab initio study**
ERKİŞİ A., SÜRÜCÜ G., Ellialtıoglu R.
Philosophical Magazine, vol.97, no.26, pp.2237-2254, 2017 (Journal Indexed in SCI Expanded)
- XXXV. **Structural phase transition, electronic, elastic, and vibrational properties of LiAl intermetallic compound: insights from first-principles calculations**
Mogulkoc Y., ÇİFTÇİ Y., Surucu G.
CANADIAN JOURNAL OF PHYSICS, vol.95, no.8, pp.691-698, 2017 (Journal Indexed in SCI)
- XXXVI. **The investigation of electronic, magnetic, mechanical, and lattice dynamical properties of PdMX (M = Cr, Fe and X = Si and Ge) ferromagnetic half-Heusler metallics: an ab initio study**
ERKİŞİ A., SÜRÜCÜ G.
MATERIALS RESEARCH EXPRESS, vol.4, no.6, 2017 (Journal Indexed in SCI)
- XXXVII. **Investigation of structural, electronic and anisotropic elastic properties of Ru-doped WB₂ compound by increased valence electron concentration**
Surucu G., Kaderoglu C., Deligoz E., Ozisik H.
MATERIALS CHEMISTRY AND PHYSICS, vol.189, pp.90-95, 2017 (Journal Indexed in SCI)
- XXXVIII. **Structural and Thermoelectronic Properties of Chalcopyrite MgSiX₂ (X = P, As, Sb)**
Kocak B., ÇİFTÇİ Y., Surucu G.
JOURNAL OF ELECTRONIC MATERIALS, vol.46, no.1, pp.247-264, 2017 (Journal Indexed in SCI)
- XXXIX. **Produce of graphene/iron pyrite (FeS₂) thin films counter electrode for dye-sensitized solar cell**
KILIÇ B., TÜRKDOĞAN S., Ozer O. C. , Asgin M., Bayraklı O., SÜRÜCÜ G., ASTAM A., EKİNCİ D.
Materials Letters, vol.185, pp.584-587, 2016 (Journal Indexed in SCI Expanded)
- XL. **First-Principles Study on the MAX Phases Tin+1Ga_nN (n=1,2, and 3)**
Surucu G., Colakoglu K., Deligoz E., Korozlu N.
JOURNAL OF ELECTRONIC MATERIALS, vol.45, no.8, pp.4256-4264, 2016 (Journal Indexed in SCI)
- XLI. **Anisotropic elastic and vibrational properties of Ru₂B₃ and Os₂B₃: a first-principles investigation**
Ozisik H., Deligoz E., Surucu G., Ozisik H. B.
MATERIALS RESEARCH EXPRESS, vol.3, no.7, 2016 (Journal Indexed in SCI)
- XLII. **First-principles investigation of LaGaO₃ and LaInO₃ lanthanum perovskite oxides**
Erkisi A., GÖKOĞLU G., Surucu G., Ellialtıoglu R., Yildirim E. K.
PHILOSOPHICAL MAGAZINE, vol.96, no.19, pp.2040-2058, 2016 (Journal Indexed in SCI)
- XLIII. **Thermo-Elastic and Lattice Dynamical Properties of Pd₃X (X = Ti, Zr, Hf) Alloys: An Ab Initio Study**
Surucu G., Colakoglu K., ÇİFTÇİ Y., Ozisik H. B. , Deligoz E.
BRAZILIAN JOURNAL OF PHYSICS, vol.45, no.6, pp.604-614, 2015 (Journal Indexed in SCI)
- XLIV. **Structural, electronic and mechanical properties of W_{1-x}TcxB₂ alloys**
Surucu G., Colakoglu K., Deligoz E., ÇİFTÇİ Y.
SOLID STATE COMMUNICATIONS, vol.171, pp.1-4, 2013 (Journal Indexed in SCI)
- XLV. **Ab-initio studies of some rare-earth borides: CeB₂, PrB₂, NdB₂, and PmB₂**
Ozisik H., Deligoz E., Colakoglu K., Surucu G.
INTERNATIONAL JOURNAL OF MATERIALS RESEARCH, vol.104, no.9, pp.858-864, 2013 (Journal Indexed in SCI)
- XLVI. **Structural and mechanical stability of rare-earth diborides**
Ozisik H., Deligoz E., Colakoglu K., Surucu G.
CHINESE PHYSICS B, vol.22, no.4, 2013 (Journal Indexed in SCI)
- XLVII. **The electronic and optical properties of MB₁₂ (M = Zr, Hf, Y, Lu) dodecaboride compounds**
Korozlu N., Surucu G.
PHYSICA SCRIPTA, vol.87, no.1, 2013 (Journal Indexed in SCI)
- XLVIII. **Structural, electronic, elastic, thermodynamic and vibration properties of TbN compound from first**

principles calculations

ÇİFTÇİ Y., Ozayman M., Surucu G., Colakoglu K., Deligoz E.

SOLID STATE SCIENCES, vol.14, no.3, pp.401-408, 2012 (Journal Indexed in SCI)

- XLIX. **Electronic, elastic and optical properties on the Zn_{1-x}MgxSe mixed alloys**
Surucu G., Colakoglu K., Deligoz E., ÇİFTÇİ Y., Korozlu N.
JOURNAL OF MATERIALS SCIENCE, vol.46, no.4, pp.1007-1014, 2011 (Journal Indexed in SCI)
- L. **Mechanical and phonon properties of the superhard LuB₂, LuB₄, and LuB₁₂ compounds**
Deligoz E., Ozisik H., Colakoglu K., Surucu G., ÇİFTÇİ Y.
JOURNAL OF ALLOYS AND COMPOUNDS, vol.509, no.5, pp.1711-1715, 2011 (Journal Indexed in SCI)
- LI. **Structural and lattice dynamical properties of Zintl NaIn and NaTl compounds**
Ozisik H. B. , Colakoglu K., Surucu G., Ozisik H.
COMPUTATIONAL MATERIALS SCIENCE, vol.50, no.3, pp.1070-1076, 2011 (Journal Indexed in SCI)
- LII. **Mechanical and lattice dynamical properties of the Re₂C compound**
Ozisik H., Deligoz E., Colakoglu K., Surucu G.
PHYSICA STATUS SOLIDI-RAPID RESEARCH LETTERS, vol.4, no.12, pp.347-349, 2010 (Journal Indexed in SCI)
- LIII. **The electronic and optical properties of Zn_{1-x}CaxSe mixed alloys**
Surucu G., Colakoglu K., Deligoz E., Korozlu N., ÇİFTÇİ Y.
SOLID STATE COMMUNICATIONS, vol.150, pp.1413-1418, 2010 (Journal Indexed in SCI)
- LIV. **Thermo-elastic and lattice dynamical properties of Rh₃Hf compound**
Surucu G., Colakoglu K., Deligoz E., Korozlu N., Ozisik H.
COMPUTATIONAL MATERIALS SCIENCE, vol.48, no.4, pp.859-865, 2010 (Journal Indexed in SCI)
- LV. **The lattice dynamical and thermo-elastic properties of Rh₃X (X = Ti, V) compounds**
Surucu G., Colakoglu K., Deligoz E., Ozisik H.
INTERMETALLICS, vol.18, no.2, pp.286-291, 2010 (Journal Indexed in SCI)
- LVI. **First-principles study of structural, elastic, lattice dynamical and thermodynamical properties of GdX (X = Bi, Sb)**
Korozlu N., Colakoglu K., Deligoz E., Surucu G.
PHILOSOPHICAL MAGAZINE, vol.90, no.14, pp.1833-1852, 2010 (Journal Indexed in SCI)

Articles Published in Other Journals

- I. **First-Principles Study on Magnetic Nature and Electronic Behavior of Silver-Based Sulfide: Ag₃MnS₄**
Sürücü G.
Süleyman Demirel Üniversitesi Fen Edebiyat Fakültesi Fen Dergisi, vol.15, no.2, pp.203-212, 2020 (National Refreed University Journal)
- II. **Anisotropic Elastic and Lattice Dynamical Properties of Cr₂AB MAX Phases Compounds**
Sürücü G.
Avrupa Bilim ve Teknoloji Dergisi, vol.15, no.1, pp.351-359, 2019 (National Refreed University Journal)
- III. **The First Principles Investigation of Structural, Electronic, Mechanical and Lattice Dynamical Properties of the B and N Doped M₂AX Type MAX Phases Ti₂AlB_{0.5}Co_{0.5} and Ti₂AlN_{0.5}Co_{0.5} Compounds**
Sürücü G., Erkişi A.
Journal of Boron, vol.3, no.1, pp.24-32, 2018 (Other Refereed National Journals)
- IV. **Enhancement in Photovoltaic Characteristics of CdS/CdTe Heterojunction**
Surucu G., Gullu H. H. , Bayrakli O., PARLAK M.
JOURNAL OF POLYTECHNIC-POLITEKNIK DERGISI, vol.20, no.4, pp.801-805, 2017 (Journal Indexed in ESCI)

Books & Book Chapters

I. Computational Modeling of Spintronic Materials

Sürücü G. (Editor)

Frontiers, Cambridge, 2021

Refereed Congress / Symposium Publications in Proceedings

- I. **Structural and Electronic Properties of Y₂Te₂O₇ Pyrochlore Oxide**
Sürücü G.
International Conference on Advanced Materials Science Engineering and High Tech Devices Applications Exhibition (ICMATSE2020), Ankara, Turkey, 2 - 04 October 2020, pp.264-265
- II. **Investigation of Mechanical Properties and the Electronic and Magnetic Behavior of Silver-Based Ferrite Chalcogenides Ag₃FeCh₄ (Ch = S and Se).**
Sürücü G.
Turkish Physical Society 36.nd International Physics Congress, İstanbul, Turkey, 1 September - 05 October 2020, pp.85
- III. **The mechanical and electronic properties of spinel oxides VX₂O₄ (X = Mn and Fe) by first principle calculations**
Yıldız B., Erkişi A., SÜRÜCÜ G.
Turkish Physical Society 35th International Physics Congress, TPS 2019, Konacik-Bodrum, Turkey, 4 - 08 September 2019, vol.2178
- IV. **First principles study of the vibrational and thermo-elastic properties of BaScO₃ perovskite oxide**
Gencer A., SÜRÜCÜ G.
Turkish Physical Society 35th International Physics Congress, TPS 2019, Konacik-Bodrum, Turkey, 4 - 08 September 2019, vol.2178
- V. **DFT study for the mechanical and electronic properties of Mg₃BH_x (x=1,4,7) compounds for hydrogen storage applications**
Gencer A., SÜRÜCÜ G.
Turkish Physical Society 35th International Physics Congress, TPS 2019, Konacik-Bodrum, Turkey, 4 - 08 September 2019, vol.2178
- VI. **An ab initio Study of Cr and Mn Doped MAX Phase TiMSiB**
YILDIZ B., Surucu G., Erkisi A.
3rd International Symposium on Multidisciplinary Studies and Innovative Technologies, ISMSIT 2019, Ankara, Turkey, 11 - 13 October 2019
- VII. **Effect of Hydrogen Doping to MgTiH₃ Perovskite Type Hydride to Enhance Hydrogen Storage Properties**
Gencer A., Surucu G.
3rd International Symposium on Multidisciplinary Studies and Innovative Technologies, ISMSIT 2019, Ankara, Turkey, 11 - 13 October 2019
- VIII. **Effects of in-situ selenization on the physical properties of CZTSe thin films**
BAYRAKLI Ö., TERLEMEZOĞLU M., GÜLLÜ H. H. , SÜRÜCÜ G., PARLAK M.
European Materials Research Society-Spring Meeting 2018, France, 18 - 22 June 2018

Supported Projects

Sürücü G., TUBITAK Project, Bor Katkılı Yüksek Performanslı İnce film Güneş hücre prototip üretimi, 2015 - 2016

Activities in Scientific Journals

FRONTIERS IN MATERIALS, Editor, 2020 - Continues

FRONTIERS IN CHEMISTRY, Committee Member, 2020 - Continues

FRONTIERS IN PHYSICS, Editor, 2020 - Continues

Aksaray University Journal of Science and Engineering, Committee Member, 2018 - Continues

Edit Congress and Symposium Activities

International Conference on Advanced Materials Science Engineering and High Tech Devices Applications Exhibition, Invited Speaker, Ankara, Turkey, 2020

Turkish Physical Society 36.nd International Physics Congress, Invited Speaker, İstanbul, Turkey, 2020

3rd International Symposium on Multidisciplinary Studies and Innovative Technologies (ISMSIT), Working Group, Ankara, Turkey, 2019

3rd International Symposium on Multidisciplinary Studies and Innovative Technologies (ISMSIT), Working Group, Ankara, Turkey, 2019

Turkish Physical Society 35.nd International Physics Congress, Working Group, Muğla, Turkey, 2019

Citations

Total Citations (WOS):527

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