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Kişisel Bilgiler

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Birimi : MOLEKÜLER BİYOLOJİ

Dahili : -

Makaleler (YOKSIS)

1 **Ab initio calculation of the structural elastic electronic and linear optical properties of ZrPtSi and TiPtSi ternary compounds**

Koc H., Yildirim A., Tetik E., Deligoz E.

Computational Materials Science,http://linkinghub.elsevier.com/retrieve/pii/S092702561200331X

2 **Ab initio calculations of the elastic electronic optical and vibrational properties of PdGa compound under pressure**

Koc H., Yildirim A., Deligoz E.

Chinese Physics B,http://stacks.iop.org/1674-1056/21/i=9/a=097102?key=crossref.df715c9ab131d62c469257c954f15502

3 **Accurate absolute free energies for ligand-protein binding based on non-equilibrium approaches**

Gapsys Vytautas, YILDIRIM AHMET, Aldeghi Matteo, Khalak Yuriy, van der Spoel David, L. de Groot Bert

Communications Chemistry,http://dx.doi.org/10.1038/s42004-021-00498-y

4 **Binding of Pollutants to Biomolecules A Simulation Study**

YILDIRIM AHMET,Zhang Jin,Manzetti Sergio,Spoel David van der

Chemical Research in Toxicology,http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00189

5 **Building Quantitative Bridges between Dynamics and Sequences of SARS-CoV-2 Main Protease and a Diverse Set of Thirty-Two Proteins**

YILDIRIM AHMET, TEKPINAR MUSTAFA

American Chemical Society (ACS),http://dx.doi.org/10.1021/acs.jcim.2c01206

6 **Competing Roles of Ca2+ and Nonmuscle Myosin IIA on the Dynamics of the Metastasis-Associated Protein S100A4**

YILDIRIM AHMET, TEKPINAR MUSTAFA, Wassenaar Tsjerk A.

The Journal of Physical Chemistry B,http://dx.doi.org/10.1021/acs.jpcb.1c02096

7 **First principles study of the structural elastic electronic optical and vibrational properties of intermetallic Pd2Ga**

7 YILDIRIM AHMET,KOÇ HÜSNÜ,DELİGÖZ ENGİN

Chinese Physics B,http://stacks.iop.org/1674-1056/21/i=3/a=037101?key=crossref.4849d0fd41804ef291ba90d4dfa498e6

8 **Impact of dimerization and N3 binding on molecular dynamics of SARS-CoV and SARS-CoV-2 main proteases**

TEKPINAR MUSTAFA, YILDIRIM AHMET

Journal of Biomolecular Structure and Dynamics,http://dx.doi.org/10.1080/07391102.2021.1880481

9 **Investigation of anisotropic thermal conductivity of uniaxial and biaxial Gay Berne particles with molecular dynamics simulation**

Yildirim Ahmet, Eroglu Erol, Yilmaz Suleyman

Molecular Simulation,http://www.tandfonline.com/doi/abs/10.1080/08927022.2011.589051

10 **Molecular dynamics investigation of Helicobacter pylori chemotactic protein CheY1 and two mutants**

YILDIRIM AHMET,TEKPINAR MUSTAFA,A Wassenaar Tsjerk

Journal of Molecular Modeling,http://link.springer.com/10.1007/s00894-014-2212-x

11 **Molecular dynamics study of the effect of active site protonation on Helicobacter pylori 5 methylthioadenosine S adenosylhomocysteine nucleosidase**

TEKPINAR MUSTAFA,YILDIRIM AHMET,WASSENAAR TA

European Biophysics Journal,http://link.springer.com/10.1007/s00249-015-1067-0

12 **Numerical Determination of Thermal Diffusivity Coefficients of Some Nematic Liquid Crystals in Situ**

Yilmaz Suleyman, Yildirim Ahmet

International Journal of Thermophysics,http://link.springer.com/10.1007/s10765-009-0670-7

13 **Only a Subset of Normal Modes is Sufficient to Identify Linear Correlations in Proteins**

TEKPINAR MUSTAFA,YILDIRIM AHMET

Journal of Chemical Information and Modeling,http://pubs.acs.org/doi/10.1021/acs.jcim.8b00486

14 **Opening mechanism of adenylate kinase can vary according to selected molecular dynamics force field**

Unan Hülya,YILDIRIM AHMET,TEKPINAR MUSTAFA

Journal of Computer-Aided Molecular Design,http://link.springer.com/10.1007/s10822-015-9849-0

15 **Optical Properties of Aligned Nematic Liquid Crystals in Electric Field**

YILMAZ SÜLEYMAN,Halide Melik,Anğay Fırat,EMEK MEHRİBAN,YILDIRIM AHMET

Scientific Research Publishing, Inc.,http://dx.doi.org/10.4236/jmp.2011.24034

16 **Optical Properties of Nematic LiquidCrystal C21H27NO2S Under AC DC Electric Fields**

Emek Mehriban, Besli Nurettin, Yildirim Ahmet, Yilmaz Suleyman

Canadian Journal of Physics,http://www.nrcresearchpress.com/doi/abs/10.1139/P09-030

17 **Propagation of uncertainty in physicochemical data to force field predictions**

YILDIRIM AHMET, Ghahremanpour Mohammad Mehdi, Spoel David van der

Physical Review Research,https://journals.aps.org/prresearch/pdf/10.1103/PhysRevResearch.2.033277

18 **Properties of Organic Liquids when Simulated with Long Range Lennard Jones Interactions**

M Fischer Nina,J van Maaren Paul,C Ditz Jonas,YILDIRIM AHMET,van der Spoel David

Journal of Chemical Theory and Computation,http://pubs.acs.org/doi/abs/10.1021/acs.jctc.5b00190

19 **Statistical efficiency of methods for computing free energy of hydration**

YILDIRIM AHMET,Wassenaar Tsjerk A,van der Spoel

The Journal of Chemical Physics,http://aip.scitation.org/doi/10.1063/1.5041835

Bildiriler (YOKSIS)

1 **Ab initio calculation of the structural electronic and opticalproperties of BiTeI compound**

KOÇ HÜSNÜ,YILDIRIM AHMET

Turkish Physical Society 28th Physics Conference ,

2 **Adenilate Kinaz Proteininin Kapalı Konformasyondan Açık Konformasyona Geçişinin Moleküler Dinamik Yöntemi ile İncelenmesi**

YILDIRIM AHMET,Unan Hülya,TEKPINAR MUSTAFA

I.Ulusal Hesaplamalı Kimya Çalıştayı ,

3 **Calcimycin inhibits the conformational dynamics of the metastasis-associated protein S100A4**

YILDIRIM AHMET, TEKPINAR MUSTAFA

ISPEC 10th International Conference On Engineering & Natural Sciences ,

4 **Comparative Investigation of Normal Modes and Molecular Dynamics of Hepatitis C NS5B Protein**

YILDIRIM AHMET,TEKPINAR MUSTAFA,Asafi ms

International Physics Conference at the Anatolian Peak , https://iopscience.iop.org/article/10.1088/1742-6596/707/1/012036

5 **How Does Ligand Binding Affect the Dynamics of SARS-CoV-2 Main Protease?**

TEKPINAR MUSTAFA, YILDIRIM AHMET

ISPEC 10th International Conference On Engineering & Natural Sciences ,

6 **Investigation of helicobacter pylori 5 methylthioadenosine s adenosylhomocysteine nucleosidase ethylene glycol and trisbuffer interactions with molecular dynamics simulation**

YILDIRIM AHMET,EROĞLU EROL

Turkish Physical Society 28th Physics Conference ,

7 **Molecular Alignment of Ferroelectric Liquid Crystals byPolyimide Thin Film**

YILDIRIM AHMET,YILMAZ SÜLEYMAN

25th European Crystallographic Meeting ,

8 **Molecular dynamics of an autoantigen in multiple sclerosis**

YILDIRIM AHMET,EROĞLU EROL

Turkish Physical Society 30th Physics Conference ,

9 **Molecular dynamics simulation study on conformational behavior of carbonic anhydrase**

YILDIRIM AHMET,EROĞLU EROL

9 Turkish Physical Society 30th Physics Conference ,

10 **Molecular dynamics simulation study onconformational behavior of the neutralizing HIV antibody 2F5 fab fragment in waterand methanol**

EROĞLU EROL,YILDIRIM AHMET,Kıytak Mehmet

Turkish Physical Society 28th Physics Conference ,

11 **Moleküler Dinamik Simülasyonuyla Gay BerneParçacıklarının Isı İletim Katsayılarının Hesaplanması**

YILDIRIM AHMET,YILMAZ SÜLEYMAN

Turkish Physical Society 27th PhysicsConference ,

12 **Nematik sıvı kristallerin sonlu farklar yöntemiyle sıcaklık gradyanı ve ısıl yayınım katsayılarının belirlenmesi**

YILDIRIM AHMET,YILMAZ SÜLEYMAN

Turkish Physical Society 24th Physics Conference ,

13 **Tek Eksenli Gay Berne Parçacıklarının NPT MolekülerDinamik Simülasyonuyla İncelenmesi**

YILDIRIM AHMET,YILMAZ SÜLEYMAN

Turkish Physical Society 27th PhysicsConference ,