Mehmet Ferdi Fellah

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Pd, Ag and Rh doped (8,0) single-walled carbon nanotubes (SWCNTs): A DFT study on furan adsorption and detection. Surface Science, 2022, 715, 121939.	0.8	10
2	A Density Functional Theory study for adsorption and sensing of 5-Fluorouracil on Ni-doped boron nitride nanotube. Materials Science in Semiconductor Processing, 2022, 137, 106183.	1.9	10
3	Adsorption of SO ₂ on Wool Fiber: An Experimental and DFT Study. Journal of Natural Fibers, 2022, 19, 1366-1375.	1.7	1
4	A DFT investigation of hydrogen adsorption and storage properties of Mg decorated IRMOF-16 structure. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 641, 128510.	2.3	11
5	Hydrogen adsorption on Ni doped carbon nanocone. Diamond and Related Materials, 2022, 124, 108921.	1.8	9
6	A Density Functional Theory Study on Graphene Triple Doped with Ga, Ge, P, Si, and Al. Russian Journal of Physical Chemistry A, 2022, 96, S77-S86.	0.1	1
7	Sensing properties of propylene oxide on Pt and Pd doped graphene sheets: A DFT Investigation. Sensors and Actuators A: Physical, 2022, 344, 113726.	2.0	6
	The supramolecularly complexes of calix[4]arene derivatives toward favipiravir antiviral drug (used) Tj ETQq0 0) rgBT /Ov	erlock 10 Tf 50
8	infrared spectroscopy of adsorption and sensing. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2021, 101, 77-89.	0.9	9
9	The reduced graphene oxide/WO3: Sensing properties for NO2 gas detection at room temperature. Diamond and Related Materials, 2021, 119, 108593.	1.8	10
10	Host–guest complex properties of calix[4]arene derivatives: a DFT study of adsorption and sensing of an anticancer drug, 5-fluorouracil. Monatshefte Für Chemie, 2021, 152, 217-228.	0.9	7
11	A DFT study on Pt doped (4,0) SWCNT: CO adsorption and sensing. Applied Surface Science, 2020, 504, 144141.	3.1	73
12	Carbon nanotubes doped with Ni, Pd and Pt: A density functional theory study of adsorption and sensing NO. Surface Science, 2020, 701, 121689.	0.8	26
13	Use of silica-based homogeneously distributed gold nickel nanohybrid as a stable nanocatalyst for the hydrogen production from the dimethylamine borane. Scientific Reports, 2020, 10, 7215.	1.6	9
14	Bimetallic platinum–rhodium nanocomposites for dimethylamine borane dehydrogenation: an experimental and density functional theory study. Catalysis Science and Technology, 2020, 10, 4624-4634.	2.1	5
15	Boron and nitrogen doping in graphene: an experimental and density functional theory (DFT) study. Nano Express, 2020, 1, 010027.	1.2	19
16	A Density Functional Theory study of molecular hydrogen adsorption on Mg site in OFF type zeolite cluster. International Journal of Hydrogen Energy, 2020, 45, 34983-34992.	3.8	15
17	Acetaldehyde adsorption and detection: A density functional theory study on Al-doped graphene. Vacuum, 2020, 175, 109279.	1.6	30
18	Ga and Ge-doped graphene structures: A DFT study of sensor applications for methanol. Computational and Theoretical Chemistry, 2020, 1180, 112828.	1.1	43

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19	Composites of Platinum-Iridium Alloy Nanoparticles and Graphene Oxide for the Dimethyl Amine Borane (DMAB) dehydrogenation at ambient conditions: An Experimental and Density Functional Theory Study. Scientific Reports, 2019, 9, 15543.	1.6	7
20	Pt doped (8,0) single wall carbon nanotube as hydrogen sensor: A density functional theory study. International Journal of Hydrogen Energy, 2019, 44, 27010-27021.	3.8	41
21	Highly monodispersed palladium-ruthenium alloy nanoparticles assembled on poly(N-vinyl-pyrrolidone) for dehydrocoupling of dimethylamine–borane: An experimental and density functional theory study. Journal of Colloid and Interface Science, 2019, 546, 83-91.	5.0	20
22	Direct decarbonylation of furfural to furan: A density functional theory study on Pt-graphene. Applied Surface Science, 2017, 405, 395-404.	3.1	27
23	A density functional theory study of hydrogen adsorption on Be-, Mg-, and Ca-exchanged LTL zeolite clusters. Journal of Molecular Modeling, 2017, 23, 184.	0.8	13
24	A DFT study of hydrogen adsorption on Be, Mg and Ca frameworks in erionite zeolite. Applied Surface Science, 2017, 394, 9-15.	3.1	16
25	Adsorption of hydrogen sulfide as initial step of H2S removal: A DFT study on metal exchanged ZSM-12 clusters. Fuel Processing Technology, 2016, 144, 191-196.	3.7	49
26	A Density Functional Theory Study of NO Reduction by C3H8 Aided Selective Catalytic Reduction Method. Catalysis Letters, 2015, 145, 964-970.	1.4	1
27	Synthesis and Characterization of a New 2-{(<i>E</i>)-[(4-aminophenyl)imino]methyl}-6-bromo-4-chlorophenol and Its Complexes with Co (II), Ni (II), Cu (II), and Zn (II): An Experimental and DFT Study. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry. 2015. 45. 1337-1346.	0.6	3
28	Use of zeolites for the removal of H 2 S: A mini-review. Fuel Processing Technology, 2015, 139, 49-60.	3.7	171
29	Hydrogen adsorption on M-ZSM-12 zeolite clusters (MÂ=ÂK, Na and Li): a density functional theory study. Journal of Porous Materials, 2014, 21, 883-888.	1.3	12
30	A DFT study on the [VO]1+–ZSM-5 cluster: direct methanol oxidation to formaldehyde by N2O. Physical Chemistry Chemical Physics, 2013, 15, 13969.	1.3	7
31	A DFT Study of Ethylene Hydrogenation Reaction Mechanisms on Ni13 Nanocluster. Topics in Catalysis, 2013, 56, 789-793.	1.3	3
32	Density functional theory investigation of acetylene dehydrogenation on metal exchanged ZSM-5 clusters for initial step of carbon nanotube production. Microporous and Mesoporous Materials, 2013, 180, 102-108.	2.2	4
33	DFT Study of Direct Methanol Oxidation to Formaldehyde by N ₂ O on the [Fe] ²⁺ –ZSM-5 Zeolite Cluster. Journal of Physical Chemistry C, 2012, 116, 13616-13622.	1.5	16
34	Epoxidation of Propylene on a [Ag14O9] Cluster Representing Ag2O (001) Surface: A Density Functional Theory Study. Catalysis Letters, 2012, 142, 22-31.	1.4	10
35	CO and NO Adsorptions on Different Iron Sites of Fe-ZSM-5 Clusters: A Density Functional Theory Study. Journal of Physical Chemistry C, 2011, 115, 1940-1951.	1.5	44
36	A DFT Study of Direct Oxidation of Benzene to Phenol by N ₂ 0 over [Fe(μ-O)Fe] ²⁺ Complexes in ZSM-5 Zeolite. Journal of Physical Chemistry C, 2011, 115, 9668-9680.	1.5	26

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37	Direct oxidation of methanol to formaldehyde by N2O on [Fe]1+ and [FeO]1+ sites in Fe–ZSM-5 zeolite: A density functional theory study. Journal of Catalysis, 2011, 282, 191-200.	3.1	25
38	Epoxidation of Ethylene by Silver Oxide (Ag2O) Cluster: A Density Functional Theory Study. Catalysis Letters, 2011, 141, 762-771.	1.4	20
39	An ONIOM and DFT study of water adsorption on rutile TiO ₂ (110) cluster. International Journal of Quantum Chemistry, 2011, 111, 174-181.	1.0	10
40	C–H bond activation of methane on M- and MO-ZSM-5 (M=Ag, Au, Cu, Rh and Ru) clusters: A density functional theory study. Catalysis Today, 2011, 171, 52-59.	2.2	19
41	A density functional theory study of C–H bond activation of methane on a bridge site of M–O–M-ZSM-5 Clusters (M = Au, Ag, Fe and Cu). Microporous and Mesoporous Materials, 2011, 138, 68-74.	2.2	38
42	A density functional theory study of ethylene adsorption on Ni10(111), Ni13(100) and Ni10(110) surface cluster models and Ni13 nanocluster. Applied Surface Science, 2010, 256, 5088-5093.	3.1	23
43	Direct gas-phase epoxidation of propylene to propylene oxide through radical reactions: A theoretical study. Chemical Physics Letters, 2010, 487, 183-189.	1.2	17
44	A density functional study of 1,1,5â€ŧris(4â€dimethylaminophenyl)â€3â€methylâ€divinylene. International Journa of Quantum Chemistry, 2010, 110, 1041-1047.	³ 1.0	0
45	A Density Functional Theory Study of Direct Oxidation of Benzene to Phenol by N ₂ O on a [FeO] ¹⁺ -ZSM-5 Cluster. Journal of Physical Chemistry C, 2010, 114, 12580-12589.	1.5	28
46	Direct Methane Oxidation to Methanol by N ₂ O on Fe- and Co-ZSM-5 Clusters with and without Water: A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 3042-3051.	1.5	47
47	Oxidation of Benzene to Phenol by N ₂ O on an Fe ²⁺ -ZSM-5 Cluster: A Density Functional Theory Study. Journal of Physical Chemistry C, 2009, 113, 15307-15313.	1.5	41
48	N2O decomposition on Fe- and Co-ZSM-5: A density functional study. Catalysis Today, 2008, 137, 410-417.	2.2	58
49	Methyl-mercaptane adsorption and sensing on Fe-/Co-graphene structures: A DFT study. Turkish Computational and Theoretical Chemistry, 0, , .	0.5	0