Liste des participants par affiche (poster)
Dimanche le 02/02/2020 à 15:20 - salle 1

PA1	Abdeli imene	Comparative study by molecular modeling methods the efficiency of tea against Alzheimer disease
PA2	Abtouche soraya	Theoritical study of optical properties of new Schiff bases of photovoltaic cells design
PA3	Aggoun sihem	Structure-property relationships and QSAR modeling of Pyridine derivatives
PA4	Almi imane	QSAR investigations of series of nitobenzoxadiazole derivatives targeting human GST and identification of novel compounds
PA5	Almi zineb	Etude théorique de la réactivité de nouvelles molécules hétérocycliques
PA6	Arbia yassamina	Nouveaux complexes organométalliques à base d'Or (III) et Cu (II) : Etude théorique au niveau DFT et TD-DFT. de la stabilité à l'activité
PA7	Ardjani taki eddine	Computational study of the structure and antibacterial activity of some Carboxylic acids analogs
PA8	Azzi asma	Etude théorique de réactions de réarrangements d'epoxyalcools.
PA9	Baira khaouther	Electronic structure applications of natural orbitals for chemical valence and QTAIM
PA10	Belaidi houmam	Insights into the optical properties of Triarylboranes with strongly electron-accepting bis(fluoromesityl)boryl groups
PA11	Benabdelmoumen fatima zohra	Etude des proprieties physiques-chimiques de quelques derives de l'Imidazolidone
PA12	Benhalima nadia	The effects of electronegative substituent atoms and dihedral angles on NLO properties of hydrazine and benzohydrazide derivatives
PA13	Benhamed lakhdar	Understanding the influence of the Trifluoromethyl Group on the Chemoselectivity of [3+2] cycloadditions of thiocarbonyl S-methanides with a,b-unsaturated ketones
PA14	Benkouider imen	Étude théorique des complexes polymétalliques à base de platine
PA15	Benmoussa charif neyla	Valorisation de la biomasse par une réaction d'hydrodeoxygénation : Etude DFT et modélisation
PA16	Bouchemalla khadidja	Etude par DFT et TD-DFT de la structure et des propriétés optiques des nouveaux échafaudages fluorescentes
PA17	Boudergua samia	QSAR Modeling using artificial neural networks and drug-likeness calculations for antioxidant activity of benzofuran derivatives
PA18	Bouhadiba abdelaziz	Molecular modeling investigation of the Herbicide Cycluron interaction in β-Cyclodextrin
PA19	Boukehil ghouzala	Modélisation moléculaire des complexes des métaux de transitions et du DHA
PA20	Boussebbat wahiba	Structural and spectroscopic characterization of the p-substituted benzaldehyde thiosemicarbazones
PA21	Chachoua amina	Étude théoriquede la réaction dyotropique
PA22	Chekkal faiza	Diversité structurale des composes organométalliques avec différents ligands (IndFeCp) ; IndFeCO3 ; IndFeBenz (Étude comparative)
PA23	Dahdouh ismail	Molecular docking/dynamics studies of novel dehydroabietylamine derivatives as Acetylcholinesterase and Butyrylcholinesterase inhibitors
PA24	Deddouche	DEDDOUCHE
PA25	Dinar karim	Theoretical and spectroscopicstudy on charge transfer complexation between an antibacterialmolecule and picricacid
PA26	Djebiha fares	Host-guest interaction between Flavonoid Fisetin and β-cyclodextrin: Molecular modeling and nuclear studies
PA27	Djellala imane	Encapsulation of anti-tumoral drug emodin within cucurbit[n]uril (CB[n], n = 6, 7 and 8):A DFT calculations
PA28	Djouama rabie	Effet des Interactions Intermoléculaires Sur les Propriétés Spectroscopiques. Aspect théorique
PA29	Guermi ikram nourelhouda	Theoretical study of the redox properties of a series of Anderson Heteropolyanions
PA30	Hazhazi halima	DFT-based reactivity and QSAR modeling of 1,2,4,5-Tetrazine inhibitors

Liste des participants par affiche (poster)
Lundi le 03/02/2020 à 10:30 - salle 1

PA31	Ibersiene fatima	A preview on quadratic hyperpolarizabilities of Lanthanide Terpyridyl complexes
PA32	Karoui samiha	Etude des propriétés structurales et électroniques par la méthode (DFT et Docking Moléculaire) d'un flavonoïde "3-Méthoxy-Qurécitine"
PA33	Khaled amira	Naproxen and β-Cyclodextrin interaction: Experimental and theoretical approaches.
PA34	Khireche moncef	Structure moléculaire et électroniques des complexes mono-bi-métallique à base du ligand BDI et du groupe imido
PA35	Kouchkar khawla	Regio-and diastereoselectivity of the 1,3-dipolar cycloaddition of N-t-butyl,α-(4-trifluoromethyl)-phenyl nitrone with methacrolein. A theoretical investigation
PA36	Koudjeti samira	Theoretical study of CsO and its cation: electronic structure and spectroscopy
PA37	Lahmar soumia	Etude théorique et expérimentale de l'effet de solvant sur les propriétés électroniques et énergétiques de phénol et de l'acide benzoique
PA38	Lehraki faiza	The effect of solvent polarity on the Quantum chemical analysis of the β Carboline
PA39	Madani salim	Density functional theory studies of a new Monomer 4-(5-Mercapto-1,3,4-Thiadiazol-2-Ylimino) Pentan-2-one
PA40	Mansouri karima	Intermolecular interactions in OLZ@ME-β-CD inclusion complexes : Meticulous investigations via AIM analysis
PA41	Mecheri sabri	Theoretical investigation of the donation and backdonation of ligand in bimetallic complexes
PA42	Merabti karim elhadj	Theoretical study of some lowest electronic states of CsS
PA43	Merouani hafida	DFT Study of the synthesis of nitrogenated heterocycles of six and seven links
PA44	Midoune assia	Etude par DFT et TDDFT des propriétés structurales, électroniques, spectroscopiques et non linéaires de la molécule tétrathiafulvalène-1,3-benzothiazole
PA45	Naili noura	Bonding study and molecular orbital Analysis of phenazine ligand in vanadium complexes: A Density Functional Theory Enquiry
PA46	Nemdili hacen	Etude structural électronique et mode de liaison des complexes hétéro-polycycliques du Cu (II) :Etude en méthode DFT
PA47	Ourdjini zeyneb	Molecular docking studies of dimers of coumarins based on 1, 2, 3-Triazole Moiety as selective Carbonic Anhydrase IX inhibitors.
PA48	Rouane abderrahmane	Investigations on molecular structure, electronic properties, NLO properties, HOMO–LUMO analysis and comparison of Drug-Likeness of quercetine derivatives by quantum methods and QSAR analysis
PA49	Sadi sabrina	Theoretical study Of [4 + 2] Diels-Alder reaction between a Diene and Alkene
PA50	Saghiri khadija	Quantitative structure-activity relationship (QSAR) study of 2-Phenyl-1H-indole derivatives as antitumor agents
PA51	Sahli rabah	Theoretical investigation: NBO and MEP analysis of the α, β, and δ isomers of the octomolybdate anion [Mo8O26]4-
PA52	Soualmia fatima	Theoretical studies of the ground and excited electronic states Pt (II) complexes using density functional theory
PA53	Taib nabila	The molecular structure of bastadin 6 and its synthetic analogs: Theoretical approach
PA54	Taieb brahim	Contribution computationnelle dans l'étude de la réactivité des médicaments : cas d'Acétaminophene (Paracétamol)
PA55	Yacef rachid	Modelisation du polymere (SENSN)X (X=1,2,3,4,5)- conductivite et supraconductivite au niveau DFT.
PA56	Yahiaoui khawla	A DFT study of inclusion complex of the antioxidant agent Hydroxytyrosol and Beta-Cyclodextrin: TD-DFT, NMR and QTAIM analyses .
PA57	Yousfi youef	The effect of internal alkynes substituents on the regioselectivity of the Ruthenium-Catalyzed Azide−Alkyne Cycloaddition: A Conceptual DFT study
PA58	Zekri afef	Étude Qualitative et Quantitative des Relations-Structure-Activité d'une Série de Dérivés de Sulfonamide

Liste des participants par affiche (poster)
Dimanche le 02/02/2020 à 15:20 - salle 2

PB01	Allab Yacine	Etude théorique par DFT de nouveaux complexes de nickel (II) avec de nouveaux dérivés de tétrazole
PB02	Allal Hamza	Removal of toxic heavy metals (Cd, Hg, Pb) from environment by borophenenanocomposites: A molecular dynamics simulation study
PB03	Ameur Anfel Saida	Investigation of some physical properties of the ternary compound Zn1-xCoxO by the TB-mBJ potential
PB04	Assas Yasmine Fatima Zohra	Storage of F2 and Cl2 molecules by the Confinement inside Boron Nitrogen Nanotube of different dimensions
PB05	Bechohra Lina Linda	Etude Ab Initio de la structure de bande electronique du nanotube de Carbone spiralé monoparoi de type zigzag (n,0)
PB06	Benadi Fatiha	Half-Heusler CaAgN compound for solar cell application: A first principles study
PB07	Benomar Sarah	First principal study of the aurivillius oxide-fluoride phase $Bi2TiO_4F_2$
PB08	Benouatas Assia	The crystal structure and conformation of (Z)-4-(Thiophen-2-Ylmethylene) Isoxazol-5(4H]-One
PB09	Bensadok Raouia	Effects of Cs substitution by Rb and Na on band gap and spontaneous polarization of $CsPbI_3$ compound
PB10	Bouchrabine Djihed	Complexes de métaux de transition diazométhines : structure, caractérisation spectroscopique, calcul théorique et investigation électrochimique.
PB11	Boulebda Hichem	Theoretical prediction of Electronic and Magnetic properties of new ferromagnetic full-Heusler alloys Rh_2MnQ (Q=Si, Al)
PB12	Bouzaheur Amal	Etude computationnelle des propriétés optiques non linéaires de dérivés du bithiophène
PB13	Charrouf Hadjer	First-principles study of Elastic, Electronic and optical properties in Sc-doped YN alloys
PB14	Cheriet Abderahman	Theoretical study of the structural and electronic properties of Cesium-Thallium halide Perovskite materials
PB15	Dilmi Toufik	Study of the electronic and structural properties of compounds InX(X=As, Sb,P)
PB16	Dziri Fatima	Couplage ab-initio calphad pour l'étude des propriétés structurales, élastiques et thermodynamiques du système Ga-Sr
PB17	Gueffaf Hamza	First-principle study of structural, electronic, elastic and optical properties of AVO_4 (A= Bi and Y)
PB18	Hadjadj aoul Ratiba	Theoretical approach of the antioxidant activity of essential oil of mint: the case of Mentha x piperita, in gaz and in solution.
PB19	Kara zaitri Lamia	Importance of Furan, Thiophene and Thiazole Moieties as p-linkers in Push-Pull Imino-dyes. A Computational investigation
PB20	Khenchoul Salah	Theoretical investigation of the structural, electronic and magnetic properties of Chloride perovskite RbFeCl3
PB21	Koribaa Imen	Structural, electronic and optical properties of the Bi0.5K0.5TiO3 compound; first principles investigation

Liste des participants par affiche (poster)
Lundi le 03/02/2020 à 10:30 - salle 2

PB22	Laissaoui Naima	Etude DFT de complexes de Platine (IV) et Palladium (II) avec le Métronidazole
PB23	Maabed Said	First principle DFT modelling of elastic, electronic and optical properties of the ternary alkali metal Copper pnectides A_2CuPn(A=Na, K and Pn=P, As).
PB24	Madkour Kamolia	Étude théorique d'un composé dopé Zn-Cd / TiO_2 –anatase: Étude comparative.
PB25	Mansouri Hadjer	Rationalization of the Antiradical Activity of Carotenoids using the Free-electron donator acceptor map model
PB26	Medjani Meriem	Etude cristalline, spectroscopique et analyse de la surface de Hirshfeld du 4,6-dichloro-5-methylpyrimidine comparées aux résultats théoriques
PB27	Merzoug Loubna	Effet de la relaxation orbitale sur le calcul du descripteur de réactivité
PB28	Nassar Meriem	Theoritical study of the photocatalytic performance in substituted lindqvist polyoxometalate [VxM6-xO19]n-
PB29	Ouakkaf Amira	XRD, FT-IR spectra and DFT vibrational analysis of 2-Amino-3-carboxypyrazin-1-ium nitrate monohydrate
PB30	Sada Sarah	Ab initio study on elastic and mechanical properties of B1-xScxN alloys in zinc blend structure
PB31	Sadok cherif Halima	Étude des propriétés de la structure électronique du composé full Heusler Co2HfGa en utilisant la GGA et la MBJ-GGA
PB32	Samsar Djamila	Theoretical Studies Of Linear And Non-Linear Optical Properties Of Substituted Bis-TTF Systems
PB33	Seghir Imene	2D-Qsar modeling of Telomerase inhibition by 1,4 diazine derivatives
PB34	Smain Tahar	Investigation of structural, electronic and lattice Dynamical properties of LaMgNi4 and Its hydrides for hydrogen storage applications
PB35	Souleh Kouider	Ab initio calculation of physical properties of Zn1-xCoxO diluted magnetic semiconductors
PB36	Touhami Hana	DFT and Experimental study on the physical properties of p semiconductor oxides Ni1-xKxO for thermoelectric and sensor applications.
PB37	Touil Zoulikha	Etude des propriétés structurales, électroniques des composés ternaire en phase chalcopyrite CuGaX2(X=S, Se)
PB38	Zaater Sihem	Etude de nouveaux complexes de palladium (II) et de platine (II) avec le sulfaméthoxazole: Corrélation entre la théorie et l'expérience.
PB39	Zerizer Mohamed Amine	Complexe Tétra-M(I) (M = Cu, Ag et Au) lié un connecteur tétra-alcynyle pyrène : Etude en méthode DFT
PB40	Zerrouki Karima	Synthesis, crystal structure, Hirshfeld surface analysis and DFT studies of an Hydrogen-Bonded dinuclear Nickel 8-Hydroxyquinoline complex
PB41	Zouchoun Fairouz	Etude théorique de complexes sandwiches binucléaires homogènes et hétérogènes de métaux de transition [M(Fv)]2 (M = Ti, V, Cr, Mn, Fe et Fv = Fulvalène)