

## Fișă de autoevaluare

alcătuită în conformitate cu prevederile fișei de evaluare generală a standardelor universității, Anexa 1

### I.I. Activitatea de cercetare ..... 612.3 puncte

#### 1. Articole științifice publicate *in extenso* în reviste cotate Web of Science cu factor de impact:

- [1] **D. Maftei**, G. Zbancioc, I. Humelnicu, and I. Mangalagiu, *Conformational Effects on the Lowest Excited States of Benzoyl-Pyrrolopyridazine: Insights from PCM Time-Dependent DFT*, *J. Phys. Chem. A*, 2013, **117**(15), 3165–3175, DOI: 10.1021/jp311396m  
.....  $(60 \times 2.775 + 25) / 4 = 47.87$
- [2] **D. Maftei**, D. Mantu, and V. Bejan, *Crystal structure of 8-(4-Methylbenzoyl)benzo [5,6] isoindolo [1,2-a] phthalazine-9,14-dione*, *Rev. Chim.*, 2013, **64**(3), 301–303  
.....  $(60 \times 0.677 + 25) / 3 = 21.87$
- [3] **D. Maftei**, I. V. Asaftei, I. Sandu, L. R. Manea, L. M. Bîrsă, and K. Earar, *Conversion of Industrial Feedstock mainly with Butanes and Butenes over HZSM-5 and Zn/HZSM-5 (nitrate) Catalysts*, *Rev. Chim. (Bucharest)*, 2015, **66**(5).  
.....  $(60 \times 0.677 + 25) / 6 = 10.94$
- [4] L. Odochian, C. Moldoveanu, and **D. Maftei**, *TG–FTIR study on thermal degradation mechanism of PTFE under nitrogen atmosphere and in air. Influence of the grain size*, *Thermochimica Acta*, 2014, **598**, 28 – 35, DOI: 10.1016/j.tca.2014.10.023  
.....  $(60 \times 2.105 + 25) / 3 = 50.43$
- [5] A. Fifere, N. Marangoci, S. Maier, A. Coroaba, **D. Maftei**, and M. Pinteala, *Theoretical study on  $\beta$ -cyclodextrin inclusion complexes with propiconazole and protonated propiconazole*, *Beilstein Journal of Organic Chemistry*, 2012, **8**, 2191–2201, DOI: 10.3762/bjoc.8.247  
.....  $(60 \times 2.801 + 25) / 6 = 32.18$
- [6] D. Mantu, **D. Maftei**, D. Iurea, C. Ursu, and V. Bejan, *Synthesis, structure, and in vitro anticancer activity of new polycyclic 1,2-diazines*, *Medicinal Chemistry Research*, 2013, **11**, 1–7, DOI: 10.1007/s00044-013-0878-8  
.....  $(60 \times 1.612 + 25) / 4 = 30.43$

- [7] M. Zaharia, S. Jurcoane, **D. Maftei**, A. Pui, C. Dumitras-Hutanu, and R. Gradinaru, *Yeast biodegradation of some pesticide dinitrophenols*, *Romanian Biotechnological Letters*, 2013, **18**(2), 8144–8151.  
.....  $(60 \times 0.351 + 25) / 6 = 7.67$
- [8] M. Zaharia, **D. Maftei**, C. Dumitras-Hutanu, P. Aurel, Z. Lagobo, O. Pintilie, and R. Gradinaru, *Biodegradation of pesticides DINOCAP and DNOC by yeast suspensions in a batch system*, *Revista de Chimie*, 2013, **64**(4), 388–392.  
.....  $(60 \times 0.677 + 25) / 7 = 9.37$
- [9] D. Mantu, D. Maftei, D. Iurea, and V. Bejan Antoci, *Crystal Structure of Ethyl 5,10-dioxo-5,10-dihydrobenzo[f]pyridazino[6,1-a]isoindole-11-carboxylate*, *Rev. Chim.*, 2012, **63**(12), 1239–1242  
.....  $(60 \times 0.538 + 25) / 4 = 17.32$
- [10] D. Ivanov, **D. Maftei**, and M. Constantinescu, *Maleamic acids cyclodehydration with anhydrides. DFT study in the gas phase and solution*, *Revue Roumaine de Chimie*, 2011, **56**(2), 89–95.  
.....  $(60 \times 0.418 + 25) / 3 = 16.69$

## 2. Articole științifice publicate în volumele conferințelor (indexate BDI)

- [1] G. Zbancioc, C. Moldoveanu, **D. Maftei**, V. Antoci, I. Mangalagiu, *Synthesis and XRD structure elucidation of new fluorescent pyrrolo-imidazole*, *Acta Chemica Iasi*, 2013, **21**(2) (supplement), 39, DOI:10.2478/achi-2013-0012  
.....  $15 / 5 = 3.00$
- [2] **D. Maftei**, D. C. Sergentu, I. Humelnicu, I. Mangalagiu, *Vibronic structure and intramolecular charge transfer character of the lowest singlet excited state in indolizine and azaindolizines: insights from theory*, *Acta Chemica Iasi*, 2013, **21**(2) (supplement), 58, DOI:10.2478/achi-2013-0012  
.....  $15 / 4 = 3.75$
- [3] D. Isac, **D. Maftei**, I. Humelnicu, *Contributions to the Thermal Degradation Mechanism under Nitrogen Atmosphere of PTFE by TG-FTIR Analysis. Influence of the Particle Size*, *Acta Chemica Iasi*, 2013, **21**(2) (supplement), 59, DOI:10.2478/achi-2013-0012  
.....  $15 / 3 = 5.00$
- [4] L. Odochian, C. Moldoveanu, **D. Maftei**, , *Computational (PCM TD-DFT) study of the first electronic transitions in cis and trans isomers of azobenzene and of some derivatives*, *Acta Chemica Iasi*, 2013, **21**(2) (supplement), 68, DOI:10.2478/achi-2013-0012  
.....  $15 / 3 = 5.00$

**9. Contracte de cercetare științifică în instituții academice (universități, institute ale Academiei Române, institute naționale de cercetare, institute de cercetare din străinătate, alte categorii de institute academice)**

- [1] Membru în echipa de cercetare, Grant PN-II-RU-TE-2011-3-0010, *New imidazole derivatives – from ionic liquids to N-heterocyclic carbenes – with potential practical applications*, oct. 2011–oct. 2014, 750000 RON, director Lector. dr. Costel Moldoveanu.

.....  $((750000/500000) \times 50)/6 = 12.50$

- [2] Membru în echipa de cercetare, Grant PN-II-IDEI-PCCE-239 9/2010, CNCSIS 239, *O noua generație de paradigme în magnetismul molecular și știința materialelor. Anizotropia magnetică în unități complexe, sisteme supramoleculare și la nano-scală*, 2010–2013, 377222 RON, director Conf. dr. Ionel Humelnicu.

.....  $(377222/500000 \times 50)/2 = 18.86$

**12. Citări și recenzii ale lucrărilor științifice (excl. autocitări)**

Articol citat: **D. Maftei**, G. Zbancioc, I. Humelnicu, and I. Mangalagiu, *Conformational Effects on the Lowest Excited States of Benzoyl-Pyrrolopyridazine: Insights from PCM Time-Dependent DFT.*, *J. Phys. Chem. A*, 2013, **117**(15), 3165–3175, DOI: 10.1021/jp311396m:

- Carlo Adamo, Tangui Le Bahers, Marika Savarese, Liam Wilbraham, Gregorio García, Ryoichi Fukuda, Masahiro Ehara, Nadia Rega, Ilaria Ciofini, *Exploring excited states using Time Dependent Density Functional Theory and density-based indexes*, *Coordination Chemistry Reviews*, aprilie 2015, *in press*, DOI: 10.1016/j.ccr.2015.03.027

.....  $(10+20 \times 12.098)/4 = 62.99$

- Singh, V. B., *Spectroscopic signatures and structural motifs in isolated and hydrated theophylline: A computational study*, *RSC Advances*, 2015, **5** (15), 11433-11444. DOI: 10.1039/c4ra15430d

.....  $(10+20 \times 3.708)/4 = 21.04$

- Srivastava, S.K., Singh, V.B., *Spectroscopic signatures and structural motifs in isolated and hydrated serotonin: A computational study*, *RSC Advances*, 2015, **5** (36), 28141-28157. DOI: 10.1039/c5ra00827a

.....  $(10+20 \times 3.708)/4 = 21.04$

- Cha, W.-Y., Lim, J.M., Park, K.H., Kitano, M., Osuka, A., Kim, D., *Two modes of photoinduced twisted intramolecular charge transfer in meso-arylaminate subporphyrins*, *Chemical Communications*, 2014, **50** (62), 8491-8494. DOI: 10.1039/c4cc02368d

.....  $(10+20 \times 6.718)/4 = 36.09$

- Wang, J., Li, M., Qi, D., Shen, W., He, R., Lin, S.H., *Exploring photophysical properties of metal-free coumarin sensitizers: An efficient strategy to improve the performance of dye-sensitized solar cells*, *RSC Advances*, 2014, **4** (96), 53927-53938. DOI: 10.1039/c4ra07904c  
..... (10+20x3.708)/4 = **21.04**
- Singh, V.B., *Spectroscopic signatures and structural motifs in isolated and hydrated caffeine: A computational study*, *RSC Advances*, 2014, **4** (101), 58116-58126. DOI: 10.1039/c4ra09749a  
..... (10+20x3.708)/4 = **21.04**

Articol citat: A. Fifere, N. Marangoci, S. Maier, A. Coroaba, **D. Maftei**, and M. Pinteala, *Theoretical study on  $\beta$ -cyclodextrin inclusion complexes with propiconazole and protonated propiconazole*, *Beilstein Journal of Organic Chemistry*, 2012, **8**, 2191–2201, DOI: 10.3762/bjoc.8.247:

- Ravera, M., Gabano, E., Bianco, S., Ermondi, G., Caron, G., Vallaro, M., Pelosi, G., Zanellato, I., Bonarrigo, I., Cassino, C., Osella, D., *Host-guest inclusion systems of Pt(IV)-bis(benzoato) anticancer drug candidates and cyclodextrins*, *Inorganica Chimica Acta*, 2015, **432**, 115-127 DOI: 10.1016/j.ica.2015.03.039  
..... (10+20x2.041)/6 = **8.47**
- Leila, L., Fatiha, M., Eddine, K.D., Leila, N., *Investigation of the inclusion processes of N-acetyl-4-aminophenol with Me- $\beta$ -cyclodextrin: A computational study*, *Journal of the Taiwan Institute of Chemical Engineers*, 2014, **45**, 387-392 DOI: 10.1016/j.jtice.2013.07.009  
..... (10+20x2.637)/6 = **10.46**
- Begel, S., Puchta, R., Van Eldik, R., *Host-guest complexes of calix[4]tubes - Prediction of ion selectivity by quantum chemical calculations VI*, *Journal of Molecular Modeling*, 2014, **20** (4), art. no. 2200 DOI: 10.1007/s00894-014-2200-1  
..... (10+20x1.867)/6 = **7.89**
- Begel, S., Puchta, R., Van Eldik, R., *Host-guest complexes of mixed glycol-bipyridine cryptands: Prediction of ion selectivity by quantum chemical calculations, part V*, *Beilstein Journal of Organic Chemistry*, 2013, **9**, 1252-1268 DOI: 10.3762/bjoc.9.142  
..... (10+20x2.803)/6 = **11.01**
- Minea, B., Nastasa, V., Moraru, R.F., Kolečka, A., Flonta, M.M., Marincu, I., Man, A., Toma, F., Lupse, M., Doroftei, B., Marangoci, N., Pinteala, M., Boekhout, T., Mares, M., *Species distribution and susceptibility profile to fluconazole, voriconazole and MXP-4509 of 551 clinical yeast isolates from a Romanian multi-centre study*, *European Journal of Clinical Microbiology and Infectious Diseases*, 2014, **34** (2), 367-383, DOI:

10.1007/s10096-014-2240-6

.....  $(10+20 \times 2.544)/6 = 10.15$

- Neamtu, A., Marangoci, N., Harabagiu, V.,  *$\beta$ -cyclodextrin/propiconazole complexes probed by constraint free and biased molecular dynamics simulations*, *Revista de Chimie*, 2013, **64** (5), 502-508

.....  $(5+10 \times 0.677)/6 = 1.96$

Articol citat: D. Mantu, D. Maftei, D. Iurea, and V. Bejan Antoci, *Crystal Structure of Ethyl 5,10-dioxo-5,10-dihydrobenzo[f]pyridazino[6,1-a]isoindole-11-carboxylate*, *Rev. Chim.*, 2012, **63**(12), 1239–1242:

- Antoci, V., Mantu, D., Cozma, D.G., Usru, C., Mangalagiu, I., *Hybrid anticancer 1,2-diazine derivatives with multiple mechanism of action. Part 3 [4,5], Medical Hypotheses*, 2014, **82** (1), 11-15 DOI: 10.1016/j.mehy.2013.10.024

.....  $(10+20 \times 1.152)/4 = 8.26$

Articol citat: M. Zaharia, **D. Maftei**, C. Dumitras-Hutanu, P. Aurel, Z. Labogo, O. Pintilie, and R. Gradinaru, *Biodegradation of pesticides DINOCAP and DNOC by yeast suspensions in a batch system*, *Revista de Chimie*, 2013, **64**(4), 388–392:

- Pantazi, M., Stefan, D.S., Constantinescu, R., Anghel, R., Meghea, A., Vasilescu, A.M., *Comparative study on the enzymatic biodegradation of synthetic and tanned leather wastes*, *Revista de Chimie*, 2014, **65** (2), 233-236

.....  $(5+10 \times 0.677)/6 = 1.96$

- Zaharia, M., Borhan, A., Gherca, D., Pui, A., Gradinaru, R., Zbancioc, G., Drochioiu, G., *Study on the mechanism of ferrite-induced dinitrophenol photodegradation*, *European Journal of Mass Spectrometry*, 2014, **20** (2), 193-197 DOI:10.1255/ejms.1267

.....  $(10+20 \times 1.165)/6 = 5.55$

Articol citat: **D. Maftei**, D. Mantu, and V. Bejan, *Crystal structure of 8-(4-Methylbenzoyl)benzo [5,6] isoindolo [1,2-a] phthalazine-9,14-dione*, *Rev. Chim.*, 2013, **64**(3), 301–303:

- Antoci, V., Mantu, D., Cozma, D.G., Usru, C., Mangalagiu, I., *Hybrid anticancer 1,2-diazine derivatives with multiple mechanism of action. Part 3 [4,5], Medical Hypotheses*, 2014, **82** (1), 11-15 DOI: 10.1016/j.mehy.2013.10.024

.....  $(10+20 \times 1.152)/4 = 8.26$

Articol citat: M. Zaharia, S. Jurcoane, **D. Maftei**, A. Pui, C. Dumitras-Hutanu, and R. Gradinaru, *Yeast biodegradation of some pesticide dinitrophenols*, *Romanian Biotechnological Letters*, 2013, **18**(2), 8144–8151:

- Zaharia, M., Borhan, A., Gherca, D., Pui, A., Gradinaru, R., Zbancioc, G., Drochioiu, G., *Study on the mechanism of ferrite-induced dinitrophenol photodegradation, European Journal of Mass Spectrometry*, 2014, **20** (2), 193-197 DOI:10.1255/ejms.1267

.....  $(10+20 \times 1.165)/6 = 5.55$

#### 15. Editor/Membru în Editorial Board & Advisory Board

Web Edition Editor *Acta Chemica Iasi* ..... **10 puncte**

#### 16. Premii internaționale obținute printr-un proces de selecție

- C. Moldoveanu, D. Astefanei, **D. Maftei**, Ghe. Zbancioc, I. Stoian, I. Mangalagiu, *New imidazole based ionic liquids, European Exhibition of Creativity and Innovation EUROINVENT, Iasi 12 - 14 May 2011 (Innovative Researches R.29.) - Diploma of Excellence.*

.....  $100/6 = 16.66$

#### 19. Participări la manifestări științifice

Membru în comitetul de organizare a *Colocviului Franco-Român de Chimie Medicală*, edițiile a 2-a (2012) și a 3-a (2014) .....  $2 \times 15 = 30$  puncte

10 iunie 2015

Asist. univ. dr. **Dan Maftei**