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[Certificate of attendance]



Dr. Ammar Boukhari

Participated in the conference with the report

**"Structural, electronic and optical properties of
 CdLiF_3 and CdLiCl_3 halide perovskites using
first-principles calculation"**

Director of Institute of Physics
of the National Academy of Sciences of Ukraine,



 M.V. Bondar

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**INTERNATIONAL RESEARCH
AND PRACTICE CONFERENCE
“NANOTECHNOLOGY
AND NANOMATERIALS”**

20-23 of August 2025

Bukovel, UKRAINE

Abstract book

The International research and practice conference “Nanotechnology and nanomaterials” (NANO-2025). Abstract Book of participants of the International research and practice conference, 20–23 August 2025, Bukovel. Edited by Dr. Olena Fesenko. – Kyiv: , 2025. – P. 592.

This book contains the abstracts of contributions presented at the International research and practice conference “Nanotechnology and Nanomaterials” (NANO-2025).

The NANO-2025 Conference was organized by the Institute of Physics of NAS of Ukraine with the participation of the University of Tartu (Estonia), the Uzhhorod National University, University of Turin (Italy) and Pierre and Marie Curie University – Paris 6 (France).

NANO-2025 is the 13th conference in the series of NANO-conferences initiated by the Institute of Physics of NAS of Ukraine in 2012 in the framework of FP7 Nanotwinning project. From year to year, they attract more attention and participants. In 2012, the first meeting was held in the format of International Summer School for young scientists «Nanotechnology: from fundamental research to innovations». The 2013 and 2014 conferences were organized in conjunction with the International Summer Schools for young scientists under the same title. In 2013, this event was attended by more than 300 scientists, in 2014-2017, 450 scientists took part and in 2018 it gathered above 650 participants. In 2021 conference was attended by more than 700 scientists from Ukraine, Poland, Italy, Estonia, France, Austria, Germany, Greece, Turkey, USA, Romania, Moldova, Czech Republic, Taiwan, Lithuania, Egypt, India, Algeria, Indonesia and other countries. In 2021 - 2024 the Organizer Committee has received more than 800 application forms from about 25 countries of the world each years.

The NANO-2025 conference brought together leading scientists and young researchers from many countries of the world. This year its topics were as follows: Nanobiotechnology for health-care; Nanochemistry and biotechnology; Nanocomposites and nanomaterials; Nanooptics and photonics; Nanoplasmonics and surface enhanced spectroscopy; Nanoscale physics; Nanostructured surfaces; Physico-chemical nanomaterials science.

This year, the conference is organized with the support of the project “Knowhow Communities for Accelerating RTI Transfer in the Danube Region” (RTIT>>), DRP0200330.

Website of the Nano-2025 conference: <http://nano-conference.iop.kiev.ua>

Welcome to International Conference «NANOTECHNOLOGY AND NANOMATERIALS»!

It is my great pleasure to welcome all participants of the International Conference “Nanotechnology and Nanomaterials” (NANO-2025), which will take place in Bukovel, in the Ukrainian Carpathians, from August 20 to 23, 2025. This event is designed to foster scientific dialogue and collaboration among researchers from diverse fields working at the forefront of nanoscience and nanotechnology.

Since its inception in 2012, the NANO Conference series has become a prominent platform in Ukraine and beyond for sharing cutting-edge research and applications in nanotechnology. Each year, it brings together experienced and early-career scientists alike, offering unique opportunities to learn from internationally renowned experts and to engage in discussions on emerging scientific topics in the field.

Our previous International Conferences and Summer Schools received positive feedback from international experts and from the media. Now we are holding the 13th such Conference, for which we are deeply grateful to its indefatigable initiator and organizer, Dr. Olena Fesenko and all members of her team, as well as to the universities and institutes that are co-organizing this event.

This year, the conference will be held in a hybrid format, welcoming participants both in person and online. We are pleased to have received over 600 registrations from researchers representing more than 30 countries. The thematic program covers a broad spectrum of topics including physico-chemical nanomaterials science, nanobiotechnology for health care, nanoscale physics, nanoplasmonics and nanooptics and photonics, nanostructured surfaces, nanocomposites, and microscopy of nano-objects.

In today’s world, international scientific cooperation holds special significance. Beyond advancing research, it helps build bridges across borders and contributes to overcoming global challenges, fostering peace and understanding. This is of particular importance now for Ukraine and for many other nations.

I wish all participants a productive and inspiring conference—one that expands knowledge, strengthens collaboration between academia and research institutions, and lays the groundwork for impactful innovations in nanoscience and nanotechnology.

May peace accompany us all, and may our scientific research continue!



**President of the National Academy
of Sciences of Ukraine**

Anatoly Zagorodny

Wear resistance of nanostructured layer alloyed with boron and nitrogen on steel 45 surface

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One of the methods for improving the quality and reliability of modern machinery is surface nanostucturization of the components to enhance their wear resistance. It could be achieved, among others, by mechanical-pulse treatment (MPT) of the surface due to its severe plastic deformation [1].

The influence of alloying with boron and nitrogen of the surface nanostructured layer on steel 45 during MPT on its wear resistance was investigated in this paper and compared with the unalloyed one. The nanocrystalline layers with ferrite-austenite structures of different depths and microhardness (150 μm and 9.2 GPa alloyed layer; 200 μm and 9.6 GPa unalloyed layer) were formed on the steel 45 surface. The grain sizes of ferrite and austenite on the steel top surface were as follows: 22.5 and 31.5 nm with alloying and 28.5 and 75.5 nm without alloying. It was also detected that the wear resistance of the specimen owing nanocrystalline layer alloyed with boron and nitrogen rises by 1.6–1.7 times compared with it without alloying. This was explained by the change the electrode potential of the surface, and its susceptibility to the formation of secondary structures on the friction faces such as FeO , Fe_2O_3 , and Fe_3O_4 , besides high microhardness of the strengthened layer. Therefore, the formation of the strengthened layer on steel surface during MPT with its simultaneous alloying is an important factor for enhancing the wear resistance of the surface layer and substantially affects its tribological characteristics.

1. Kyryliv V, Maksymiv O., Gurey V, et al. The mode deformation effect on surface nanocrystalline structure formation and wear resistance of steel 41Cr4 // *Coatings*.-2023.-13, N 2.-Article No. 249.

A

Abaloszew A.	481
Abaloszewa I.	481
Abramenko L.O.	37
Afanasieva T.V.	400, 511
Afanasieva T.V.	511
Akimov V.	56
Akopian V.	38
Akopova O.V.	220
Aksimentyeva O.	419
Aksimentyeva O. I.	22, 102, 422
Al-Ateqi A.	458
Aleksandrova A.	208
Alekseev O.M.	374
Alekseev S.O.	374, 531
Aleman Arrebola L.J.	154
Aliksandrov M.A.	350, 440
Allali D.	68
Amari R.	68
Amirulloieva N.	205
Andrarczyk T.	532
Andriash H.S.	233
Andriichuk Y.	451
Anhelov M.	218
Aniolek K.	200
Antonin S.V.	501
Antoniuk R.I.	399
Antonov V.N.	493
Apanasenko V.	189
Apopii V.	439, 444
Apostolakis A.	458
Ardanova L.I.	355
Artyukhov A.E.	90, 91, 93
Artyukhova N.O.	90, 91, 93
Atabayev T.	299
Atamas O.	228
Auinger M.	76
Avramenko V.V.	206

B

Babayevska N.V.	367
Babenko N.M.	223
Babich L.G.	226
Babichuk I.S.	339, 342
Babichuk I.V.	339, 342
Babkina N.V.	19
Babsky A.M.	239
Babuka T.	485
Babutina T.	88

Bachynskiy O.	98
Bajana O.	500
Bakhmat V.A.	284, 294
Balabai R.M.	335
Balaban O.	17
Balin K.	407, 409
Baraban L.	243, 294
Barabash M.Yu.	496
Barabashko M.	194
Baran M.M.	340, 341
Baranchykov Z.	505
Barbash V.	210
Barbash V.A.	124
Barlas T. R.	208, 412
Barvinko M.A.	176
Barylski A.	200
Bashev V.F.	46, 64, 305
Basnukaeva R.	194
Batentschuk M.	349
Bavdys M.	460
Bazylyak L. I.	161
Bednarchuk T.	18
Behdai A.O.	57
Bekenov L.V.	493
Belarouci A.	138
Beliak Ie.V.	114
Belkina I.O.	232
Belosludtsev A.	443
Belous A.	483
Belous A.G.	113, 188, 332, 370, 500
Belyavina N.M.	59
Benrezgua E.	68
Berezhnyi O.Yu.	467
Bereznykov O.V.	39
Berezovets V.V.	300
Berezovska N.	402
Berketa K.	243
Bespalko O.V.	209
Bessarabov V.I.	57
Beygelzimer Yan.	10
Bezhubenko P.	12
Bezkrivnyi O.	194
Bezrodna T.V.	438
Bezsmertna O.	294
Bezvikonnyi O.	425, 526
Bielkina I. O.	236
Bielousova N.B.	34
Bihu R.	439
Bihun R.	444
Bilanchuk M.V.	134
Bilanych B.V.	393

- Bilanych V. 84, 134, 393, 506
 Biliak R.V. 60
 Biloivan O.A. 253
 Birchenko A.P. 65, 489
 Bischoff K. 382
 Bitinaitis I. 443
 Blashkiv O. 241
 Blazevicius D. 450
 Bochechka O.O. 121
 Bochkova G.Yu. 9
 Bodnaruk A.V. 39
 Bodul N. 486
 Bogatryyova H. 382
 Bogoslovska A. 11, 450
 Bogutska K. 218
 Bohdan L. 142, 396
 Boichuk N. 125, 392
 Boichyshyn L. 200, 407, 409
 Boichyshyn L.M. 406
 Boiko V. 505
 Bojko Yu.I. 354
 Boldyrieva O.Yu. 361, 362, 363, 365
 Bondar R.V. 315
 Bondar Yu. 75
 Bondarenko S.I. 478
 Bondarenko V. 103
 Bondarenko V.P. 307
 Bondarovych M.O. 223
 Borblik V.L. 476
 Bordun B. O. 52
 Bordun I. 135
 Bordun O. M. 52
 Boretskij V. 189
 Borisenko L.I. 364
 Borkovska L. 521
 Borkovska Yu.B. 307
 Borodinova T. 108, 412
 Borovyi M. 70
 Bortchagovsky E. 11
 Boryak O.A. 153
 Borysenko M. 28, 81, 143
 Borysenko M.V. 410
 Borysiuk A. 135
 Borysiuk V. 140, 210
 Borysiuk V.I. 53, 348
 Botvynovskyi B.O. 278
 Boudebs G. 78
 Boukhari A. 68
 Bouleklab M.C. 123
 Bovgyra O.V. 127, 144
 Bovhyra R.V. 144
 Bovtun K.I. 290
 Boychuk A.M. 100
 Boychuk T.Ya. 100
 Boychuk V.M. 16, 113
 Boyko V. 140, 210, 486
 Boyko V.V. 53, 124, 348
 Bratus O.L. 501
 Brazhnyk I.V. 306
 Breton T. 78
 Brodin O.M. 416
 Brodskii R.Ye. 345
 Brovko O.O. 282
 Brytan A.V. 366
 Budnyk O. 540
 Budnyk O.P. 426, 432, 539, 540, 534
 Budylna O. 97
 Bugaychuk S. 447
 Bulavin L.A. 480
 Bulavinets T.M. 38, 469
 Burdyny V.H. 340
 Burtsev V.V. 94
 Burylov S.V. 85
 Burylova N.V. 85
 Busko T.O. 109
 Bychko I.B. 300
- C**
- Cabal B. 151
 Caha O. 405
 Calus D. 135
 Canciani M. 258, 388
 Cebulski J. 454
 Chaban M.O. 86
 Chabanenko V.V. 481
 Chalyy D. 167, 168
 Charnyi D. 75
 Cheban L.M. 54
 Chegel V.I. 466, 470, 471
 Chepela L. 70
 Cherednichenko S.V. 194
 Cherenok S.O. 245
 Cherifi-Hertel S. 33
 Chernienko O.I. 121
 Chernyshenko V.O. 245
 Chervakov O. 312
 Chornii V. 140, 210, 356
 Chornii V.P. 53, 124, 348, 374
 Chornovol V. 353
 Chrastny V. 75
 Chudinovych O. 116

Chumak A. V.	497
Chumak H.L.	336, 361, 362, 363, 364, 371, 372
Chuprina M.O.	530
Ciemięga A.	82
Cortés Reyes M.	154
Coutelier O.	334
Csoma Z.	108
Curmei N.D.	438

D

Dan'kiv O.O.	477
Danilchenko V.E.	514
Dankiv O.O.	99
Danylenko I.M.	350
Danylenko I.O.	57
Danylenko K.	145
Danylovych H.V.	267
Danylovych Yu.V.	267
Daoud L.	78, 79, 224
Datsenko O.I.	386
Davtyan L.L.	229
Deghfel B.	68
Dekhtyar M.L.	456
Dekhtyarenko V.A.	30
Demchenko L.	333
Demchenko V.	259, 277
Demchenko V.H.	371, 372
Demchenko V.L.	3, 4, 5, 184, 286, 535
Demchenkov S.	508
Demchyna O.O.	191
Demediuk R.	56
Demianenko E.M.	214
Demydov P.V.	470, 471
Deryło-Marczewska A.	81
Destarac M.	334
Deva L.	424, 425
Dibrov V.	139
Didenko G.Yu.	273
Didenko Yu.V.	10
Didkovskiy T.M.	122
Diedkova K.	408, 411
Dikhtiaruk E.V.	410
Dimitriev O.	450
Diyuk N.V.	190, 371, 372
Diyuk V.E.	361, 362, 363, 364, 365, 371, 372
Djakin M.V.	512
Dmitrenko V.	349

Dmitrenko V.	41
Dmitriev A.I.	325,
Dmytrenko O. P.	09, 229, 238, 278
Dmytruk I.	402
Dobrovolska A.	334, 455
Dolbin A.	194
Dolgoshey V.	259, 277
Dolgoshey V.B.	286, 288, 290
Dolgov L.	408, 411
Domagala J. Z.	532
Dong Ziwen	40
Dontsova T.A.	66, 142, 156, 352, 389, 399
Doronin Yu.S.	479
Doroshchuk V.V.	160, 255
Doroshenko I. Yu.	229
Dorozinsky G.V.	466
Doskaliuk N.	451
Dovbeshko G.	525
Dovbynychuk T.	159
Drobot L.B.	301
Drozdova A.O.	229
Druzhinin A.	499
Dubey I. Ya.	268
Dubrava T.G.	223
Dubs C.	497
Dubyk K.V.	58
Dudetskaya G.	106, 129, 225
Dudetskaya G.V.	110
Dudnik O.	143
Dumych T.	224, 283
Duque C.	56
Dusheiko M.G.	389
Dutka V.S.	117, 120
Dutka Yu.V.	120
Dvornichenko A.V.	21
Dyachenko A.	81, 143
Dyakin M.V.	516
Dybkov M.V.	293
Dybko S.M.	80, 246, 293
Dzevin Ie.	514
Dzhezherya N.L.	9
Dzhezherya Yu.I.	6
Dziubenko N.	159
Dzyadevych S.	243
Dzyadevych S.V.	80, 284, 294, 466
Dzyazko Yu.S.	86, 213
Dzyuba O.I.	254
Dzyuba V.I.	309
Dzyubenko M.I.	423

E

Eliseev E.A. 31, 33
 Eliyashevskyy Y. 158
 Elmers H.-J. 532
 Evans D.R. 31
 Evans D.R. 33
 Evtukh A. 375
 Evtukh A.A. 501

F

Fainleib A.M. 196, 216
 Fandzloch M. 505
 Fatieiev D.S. 300
 Fedchenko O. 532
 Fediai V.D. 302
 Fedko M.M. 296
 Fedorchuk O.P. 188, 332, 370, 500
 Fedorenko L. 375
 Fedorus O.G. 400
 Fedorus O.H. 395
 Fedotov O. 78, 79
 Feher A. 393, 506
 Feia O. 519
 Feldii M.M. 47
 Fernández A. 151
 Ferrara A. 408, 411
 Fesenko O.M. 523, 534, 536, 537, 538,
 539, 540
 Fesych I.V. 9, 10, 39, 215
 Fialkin Ye.M. 274
 Fihurka N.V. 198
 Filep M. 84
 Firstov S. 104
 Fischer L. 169
 Fischuk O.S. 111
 Fitio V.M. 436, 442
 Fiyalka L.I. 325
 Flandorfer H. 169
 Fomina O. 56
 Forys I.S. 267
 Franciska Erdő. 538
 Frolov Yu.O. 494
 Frolova L. 13
 Furtat I. 211
 Furtat I.M. 206, 209

G

Gaevska Yu.O. 223
 Gaidai S.V. 111

Galaburda M. 81
 Galagan P.O. 46
 Galiy P.V. 309
 Gallo González J. 148
 Galtsov N. 18
 Gaponov A.M. 109
 Garbovskiy Y. 125
 Garcia-Granda Santiago 148
 Gavryushenko D.A. 515
 Gerasimchuk I.V. 491
 Gerasimchuk V.S. 491
 Get'man E.I. 355
 Gnatyuk O. 525
 Gnilit'skiy I. 398, 408, 411
 Godzierz M. 235
 Gogotsi H.G. 201
 Goltsev A.M. 223, 223
 Golz C. 208
 Gomenyuk O. 356
 Gonchar O.M. 136, 336
 Goncharova I. 457
 Goncharuk O.V. 293
 Gorbyk P.P. 193
 Gorelov B.M. 214
 Gornostai O.V. 77
 Goy A.M. 57
 Grabarczyk M. 185
 Grande D. 216
 Grankina I.I. 23
 Grazulevicius J.V. 424, 425
 Grazulevicius V.Ju. 526
 Grechanyuk I. 376
 Grechanyuk I. M. 328
 Grechanyuk M.I. 328
 Grechanyuk V. 353
 Grechanyuk V.G. 328
 Grigalevicius S. 450
 Grigoriev A.N. 515
 Grigoryeva O.P. 196, 216
 Grishchenko L.M. 336, 361,
 362, 363, 364, 365,
 371, 372
 Grivel J.-C. 128
 Grohotov V. 38
 Gruzina T.G. 246, 293
 Grygorova G. 106, 129, 232, 236, 367
 Grynko D. 11, 12
 Grynyuk I.I. 44, 62, 67, 203, 301
 Grzegory I. 446
 Gudenko J.M. 215
 Gudyma Iu.V. 24

Guichaoua D.	457
Gule E.	390
Gun'ko V.M.	410
Gunya G.M.	69
Gurevičienė V.	250
Gurin I.V.	94
Gvozдовskyy I.	382

H

Hadzaman I.	166, 171
Halechko H.M.	117
Hamalii N.V.	435
Hamalii O.V.	435
Hamamda S.	123, 356
Hanke M.	208
Haponov O. M.	238
Harbat D.	171
Harhay Kh.	17
Havii V.	92
Havrylova V.S.	122
Hellmann R.	382
Herasymchuk M.O.	288
Herrera Delgado C.	154
Herrmann C.	208
Hertel R.	33
Hertsyk O.M.	406
Hes N.L.	304
Hevko I.	398
Hirskiy Yu.	204, 348, 505
Hnatiuk K.I.	531
Hoang S.	224
Hodlevskiy H.	211
Hoi V.T.	16
Hołdyński M.	81
Holomb R.M.	329
Holyboroda S.I.	436
Honcharova L.A.	19
Honta V.A.	310
Horbatenko Yu.	194
Horbenko Yu.Yu.	22, 35, 422
Horbyk P.P.	69
Hordeeva S.O.	366
Hrankina S.S.	23
Hreb V.	181, 186, 192, 204, 518
Hrebelska Yu.V.	25, 40, 48, 69, 520
Hromova D.S.	316
Hryhorova T.V.	45
Hryn V.	523, 537
Hrytsak R.V.	47
Hrytsyna M.	517

Hrytsyna O.	517
Hubenko K.	106, 110, 129
Hubetska T.	148, 151
Hudyma A.	211
Hudzenko I.I.	470
Hula A.	460
Hurmach V.V.	221
Hurova D.	18
Huseinova K.E.	296
Hushynets R.I.	449
Hutsul Kh.R.	73, 74, 302

I

Iakovlev V.E.	514
Iatsenko A.	97
Ievtushenko A.I.	325
Ignatenko O.M.	48, 69
Iilashchuk M.I.	326
Ilchenko M.M.	268
Ilchuk H.A.	384
Ilkiv B.I.	380
Ilkovich S.	143
Illing R.	243, 294
Ilyin P.P.	109
Ingram A.	165
Inshina O.I.	304
Irodov D.M.	237
Isaiev M.	70
Ishchenko O.	143
Iukhymenko N.	373
Iukhymenko N.	295
Iurzhenko M.V.	4, 184, 259, 277, 288, 290, 535
Ivakh M.S.	133
Ivanchenko S.	536
Ivanchenko S.E.	80
Ivanenko K.O.	40
Ivanenko K.O.	48
Ivanichok N.Y.	113
Ivaniuk K.B.	431
Ivanov O.V.	308
Ivanova N.N.	240
Ivashkiv V.R.	403

J

Janićijević Ž.	294
Jeżowski A.	194
Jobolda I.	13
Kabat O.S.	199

- Kachalova N.M. 254
 Kachkovsky O.D. 278
 Kachorovska O. 486
 Kachurak Y.M. 133
 Kaidash O.M. 344
 Kalchenko V.I. 226
 Kaleinikova O. 241
 Kalenyuk O. A. 41, 404
 Kalinina T.V. 46
 Kalita V. 483
 Kalynets N.I. 99
 Kamarchuk G.V. 479
 Kamenskyh D.S. 4, 340
 Kanibolotska L. 424, 425
 Kanibolotsky D.S. 14
 Kanibolotsky O. 424, 425
 Kanyuk M.I. 229
 Kapatsila S.M. 195
 Kapitanchuk O.L. 260, 415
 Kapp M. 152
 Kaptay G. 169
 Kapustianyk V. 158
 Karabanova L.V. 19
 Karachevtsev V.A. 153
 Karachevtseva L.A. 26, 29
 Karashu V.R. 221
 Karandas Ya.V. 464
 Karbivski V.L. 441
 Karbivsky V.L. 308, 337, 368, 418, 421
 Karbovnyk I. 164, 167, 168, 460
 Kareiva A. 181, 186
 Karolus M. 200, 407, 409
 Karpenko N.A. 232
 Karpenko N.O. 236
 Karpenko Yu.V. 292
 Karpets M.V. 15
 Karpov M.Ye. 128
 Kartel M.T. 26, 29, 40
 Kashirina N.I. 343
 Kashuba A.I. 384
 Kashuba I.V. 45
 Kaupuzs J. 375
 Kavok N. 106, 129
 Kavok N.S. 110, 225, 367
 Kaykan L. 482
 Kaykan L.V. 58
 Keda T. Ye. 190
 Kernosenko L. 96
 Khachatrian A. 104
 Khainakova O. 151
 Khalameida 28
 Khalameida S. 27
 Khalavka Y. 451
 Khalavka Y.B. 54
 Khaliavka T.O. 128
 Khamar O.O. 117
 Kharchenko D.O. 21
 Kharchenko O. 224, 283
 Kharchenko V.O. 21
 Kharchenko Y.V. 318, 319, 323, 324
 Khatibi G. 76, 169, 170
 Kheylomska T.O. 276
 Khodabakhshi F. 76
 Kholod P.F. 318, 319
 Khomenko D.M. 449
 Khora O.V. 214
 Khort P. 78, 79
 Khovanets' G.I. 191
 Khovavko A.I. 157, 163
 Khoverko Yu. 499
 Khrunyk D. 87
 Khrushchuk Kh. 170, 200, 407, 409
 Khutko M.M. 470, 471
 Khyzhun O. 28
 Kiose T.O. 524
 Kirian I.M. 94, 174, 182
 Kiziun O.V. 29
 Klepko V.V. 67, 130
 Kliaznika D. 297, 299
 Klimenkov O.M. 389
 Klimusheva G. 125
 Klishevich G.V. 438
 Klochkov V.K. 232, 236, 247, 248
 Klym H. 164, 165, 166, 167, 171, 172
 Klym H. 460
 Klymchuk D.O. 67
 Klymiuk M. 16
 Kniaziev S.A. 401
 Kniazieva H.O. 401
 Kobrii V. Ye. 190
 Kobrina L.V. 280
 Kobylinska N. 148
 Kobylinska N.G. 151
 Kofliuk I. M. 52
 Kogut I. 499
 Kogutyuk P.P. 59
 Kokhan I.V. 61
 Kokhan O. 84
 Kokhan S.V. 21
 Kolbasov G.Ya. 359
 Kolendo A. 373

Kolesnichenko V.	116	Korostil A.	520
Kolesnik D.	525	Korotash I.V.	105, 435, 498, 512, 516
Kolka I.	192	Korotkov K.A.	325
Kolkovska H.M.	113	Korotun A.V.	37, 420, 434, 461, 462, 465, 466, 468
Kolkovskiy P.I.	113	Korpan Ya.I.	253
Kolodiy I.V.	45	Korzh R.A.	190
Kołodziej J.	405	Kosevich M.V.	153
Kolomys O.F.	350, 440	Koshets I.	382
Kolotilov S.V.	187, 255	Kost Y.Y.	60
Kolupaev B.B.	83	Kosterin S.O.	226
Kolupaev B.S.	72	Kostetskiy A.O.	101
Kolupaev B.S.	72	Kostiv Yu.	171, 172
Koman B.	444	Kot K.V.	233
Komanicky V.	84, 134, 393, 506	Kot L.A.	432
Komashchenko Ye.O.	44, 62, 203	Kot Yu.	106, 129
Kompanets M.O.	254	Kot Yu.G.	247, 248
Konanets R.	167, 168	Kotrechko S.O.	176
Kondrat O.B.	329	Kotsiubynskiy V.	451
Kondrat O.O.	329	Kotsuybysky V.O.	16, 113
Kondratenko I.	88	Kotynska L.	27, 28
Kondratenko O.	532	Kovach V.V.	274
Kondratenko S.V.	386	Kovadlo V.P.	523, 538
Konechna P.T.	266	Koval L.I.	122
Konopelnik O.I.	102	Kovalchuk M. V.	237
Konoplyov O.M.	383	Kovalchuk M.O.	290, 535
Konovalenko A.	373	Kovalchuk O.	125
Konovalova V.	87	Kovalchuk V.I.	307
Kopa I.	71	Kovalenko L.L.	188, 332, 500
Kopach V.	451	Kovalenko M.V.	127
Kopanchuk S.	408, 411	Kovalskiy A.	455
Koplak O.	258, 388	Kovalskiy Ya.P.	117
Korchovyj A.	382	Koverya V.P.	478
Kordan V.	407, 409	Kovtun S.I.	261
Kordan V.M.	22, 397	Kozakevych R.B.	209
Kordium V.A.	237	Koziarskiy D.P.	326
Kordyuk O.	519	Koziarskiy I.P.	326
Korenchuk M.S.	253	Kozliuk D.	166
Koreniewa Ye.M.	236	Kozyrev A.V.	328
Korenivski V.	6	Kramar A.S.	111, 359
Koretska N.I.	191	Kramar O.	55
Korinenko B.V.	341	Krasuliak O.A.	156
Kormosh V.V.	134	Kravchenko V.V.	358, 360, 530
Korochkova T.Ye.	490	Kravchuk R.M.	347
Korohodska A.M.	155	Kravchun M.A.	374
Korolkov R. Yu.	420, 461, 464, 467	Kravets A.	333
Korolova D.S.	245	Kravets A.F.	6
Korolyuk O.	194	Kredentser S.	447
Koronovskyy V.E.	112	Kremer I.P.	133
Korostil A.	502	Krevsun A.V.	478
		Krivchikov A.	194

Krivoruchko V.	41	Kushnerov O.I.	46, 64
Krmela J.	90, 91, 93	Kushnir O.	164, 172, 460
Krolenko K.	356	Kushnir V.	80
Krucaite G.	450	Kusiak N.V.	193
Kruhlov I.O.	147	Kuskova N.I.	36
Krupa M.	502	Kusyak A.P.	193
Krupka O.	78, 79, 224, 283	Kutovaja V.V.	240
Krupka O.M.	412	Kutseva N.	64, 244
Kryuchyn A.A.	114	Kutsevov N.V.	222
Kryvoschapka R.V.	401	Kutsii S.A.	442
Kubisztal Yu.	407	Kuzema P.O.	153
Kubisztal Yu.	409	Kuzmych L.V.	109
Kucherenko V.O.	4	Kuzmych S.A.	109
Kucherov O.P.	331	Kuznetsov V.K.	85
Kuchmenko O.	92	Kuznietsov V.V.	470
Kuchuk O.I.	481	Kuznietsova H.	159
Kudelko K.	86, 180, 213	Kuzyk N.I.	431
Kukhareno S.A.	344	Kuzyk O.	98
Kukharskyi I.Yo.	52	Kuzyk O.V.	99, 477
Kukhtaruk N.I.	350	Kychkyruk O.	118
Kukusta D.A.	493	Kyrii S.O.	73, 302
Kulakovska A.Y.	266	Kyriienko P.I.	126
Kulbachinskiy O.A.	412	Kyrychek M.P.	34
Kulich M.P.	109, 229, 238, 278	Kyrychuk Y. T.	298
Kulich Yu.V.	270	Kyrylenko O.I.	426
Kulyk T.	25	Kyryliuk D.V.	311
Kulyk V.V.	318, 319, 320, 321, 322, 323, 324	Kyryliv V.I.	403
Kulyk Y.O.	403	Kyryliv Y.B.	403
Kulyk Yu.	200, 448	Kysil D.	429, 450
Kunakova G.	205	Kyslyi V.	521
Kunytska L.	334	Kytsya A. R.	161
Kunytskyi D.V.	3, 4, 5	Kytsya A.R.	191
Kuprin O.	398		
Kurbatsky V.P.	434, 468		
Kurgan N.A.	308, 337, 418, 421, 441		
Kurganov R.M.	344		
Kurioz Yu.I.	347, 447		
Kurmach M.M.	29, 131, 187, 255, 310, 311, 338		
Kurochka L.I.	109		
Kurowska I.	334		
Kurta S.A.	262		
Kurylenko V.S.	156		
Kuryliuk A. M.	44, 59, 62, 374		
Kuryliuk O.	295		
Kuryliuk V.	139		
Kuryliuk V.V.	361		
Kushch V.V.	15		
Kushlyk M.	453, 454, 455		
		L	
		Labudzynskyi D.O.	44, 256
		Labunets A.R.	149, 150
		Lagoda D.	13
		Lakhnik A.M.	94, 182
		Lamonova K.V.	349
		Lampeka R.D.	301
		Larina O.V.	126, 128, 131
		Laroze D.	56
		Larrubia Vargas M.A.	154
		Laun V.	63, 76
		Lauth-de Viguerie N.	334
		Lavrik R.	486
		Lavriv N.	38
		Lavrovsky C. E.	331
		Lavrynenko O.	534
		Lavrynenko O.M.	7

- Maliuta S.V. 386
 Malovanyy M. 135
 Malysh R.O. 461
 Malyshev V.Yu. 196, 346
 Malyushevskaya A.P. 36
 Mamunya Ye. 235
 Mamunya Ye.P. 136
 Mamykin S. 375, 402, 412, 532
 Mandryka A. 13
 Manilo M. 108
 Maniuk M.S. 468
 Manoryk P. 402
 Marchenko A.A. 15
 Marchenko S.V. 80, 250
 Marchuk M. 82, 87
 Margitych M.O. 274
 Mariichak O.Yu. 202
 Mariychuk R. 143
 Mariychuk R.T. 190
 Markin O.O. 24
 Markitan O.V. 214
 Markiv Yu.B. 102
 Markova N.B. 155
 Martseniuk V. 529
 Marty J-D. 334
 Martynenko I.O. 41, 404, 478
 Maruzhenko O. 235, 259
 Mashira V.A. 490
 Maslov V. 390
 Masselink W.T. 208
 Masuzawa T. 375
 Matiushyn V. M. 37
 Matsenko A.V. 328
 Matsenko O. 376
 Matsui L.Yu. 174, 182
 Matsuy V.I. 43
 Matushko I.P. 228, 336,
 346, 361, 362, 363, 365
 Matvienko Ya. 508
 Matyovka Yu. Yu. 393
 Matyshevska O.P. 301
 Matzui L.Yu. 2, 32, 34, 43, 58, 141
 Maziar D.M. 350, 440
 Mazur M.P. 385
 Mazur T.M. 385
 Mazur Y.I. 327
 Mazur Yu. 390
 Mazurenko J. 482
 Mazurenko J.S. 58
 Medvid I. 454
 Medvid I. I. 52
 Melezhyk Ye.O. 350, 440
 Melnyk I.V. 193, 341, 438
 Melnykov S.O. 431
 Melnykov V.M. 206
 Midyana G.G. 120
 Mieziientseva O. 56
 Mikhaylova H.Yu. 30, 42
 Mikhin N.P. 65, 489
 Milenin G.V. 472
 Mimura H. 375
 Minchenko O.H. 270
 Minitskyi A.V. 496
 Minya O.I. 47
 Mirnaya T. 125
 Mironov O.L. 254
 Mischanchuk O. V. 36
 Misiura A. 235, 535
 Mitina N. 17
 Mitina N.E. 239
 Mitsa O.V. 329
 Mitsa V.M. 329
 Mizeracki J. 96, 97, 116
 Moiseienko V.A. 336, 346,
 361, 362, 363, 365,
 371, 372
 Moiseienko Yu. Yu. 32
 Mokliak M. 482
 Mokliak V. 482
 Mokrinskaya O.V. 360, 530
 Molebny O. 508
 Monastyretskyi M.G. 280
 Monastyrska T.O. 94
 Monastyrsky G. 63, 76, 259,
 277, 525
 Morgunov P.V. 237
 Moroz H.V. 434
 Moroz O.I. 234
 Morozhenko V. 521
 Morozovska A.N. 31, 33, 80, 215
 Morozovsky N.V. 80, 215
 Moshchil V.E. 15
 Moskalenko V. 18
 Motuziuk O. 230
 Mrowiec-Białoń J. 82
 Mruga D.O. 294
 Mu Yingnan. 9
 Mudra E. 134
 Mudry S. 369, 448
 Murlanova T. 211
 Murlanova T.V. 206, 252
 Murmantsev A. 189

Muryi Ya. Yu.	501
Murzin D. Yu.	71
Mussabek G.	297, 299
Mykchaylova O.B.	269
Mykytyuk Z.M.	133
Myronenko O.K.	515
Mystetskyi V.	447
Mysyuk Yu.	469

N

Nabiałek A.	481
Nadtoka O.	244
Nahurskyi N.	135
Nakamura T.	380
Nashchekina O.	529
Nastych V.	521
Natsik V.	18
Naumenko A.P.	109
Navozenko O.	526
Nazarenko V.G.	347
Nazarov A.	450
Nazarov O.	429
Nechytailo B.V.	511
Nedielko M.	356
Nedielko M.S.	123
Nedilko S.	356
Nedilko S.G.	53, 62, 124, 140, 210, 348, 374
Nedozhdii O.	510
Negriyko A.M.	269
Nenchuk T.M.	309
Nesmiian K.S.	379
Nesprava V.V.	438
Netreba S.V.	330
Netyaga V.V.	325
Neuhodov Ye.	129, 225
Nikiforow K.	81
Nikolaenko A.V.	522
Nikolaenko V. A.	522
Nikolaenko T.Yu.	357
Nikolaiev K.S.	423
Nikolaiev R.O.	282
Nikolaiev S.V.	423
Nikolenko A.	158, 446
Nikolenko A.S.	350, 440
Ninyovskij V.	189
Nizhnik B.O.	197
Noskov Yu.V.	346
Noskov Yu.V.	361, 362, 364, 365
Nosova N. G.	298

Nosova N.G.	195, 198, 298
Nötzel R.	388
Novitskaya A.Ye.	498
Novytska A.Ye.	512
Nozdrenko D.	218, 230
Nykyruy L.I.	394
Nykyruy Yu.	448

O

Ohoreltseva K.A.	252
Ohtsuka M.	380
Ohulchanskyy T.Y.	430
Okunievsykyi Y. P.	149
Oleksenko L.P.	49, 50, 524
Olenchuk M.	525
Olenych I.B.	35
Oliiynyk A.O.	149, 150
Oliiynyk O.V.	496
Oliynyk Ya.	17
Olshowska N.	405
Onanko A.P.	109
Onanko Y.A.	109
Oninshchenko A.A.	110
Onishchenko A.	106, 129
Onishchenko A.I.	247, 248
Onufrijevs P.	375
Onysko M. I.	127
Opalińska A.	97, 116
Orletsykyi I.G.	326
Orlov A.K.	147
Orlova D.	529
Orovciik L.	170, 500
Oryshych D.	51, 531
Oryshych D.V.	30, 31, 42
Ostankov M.V.	223
Ostapenko R.V.	59, 62
Ostapiuk Yu.V.	239
Ovdenko V.M.	149, 150
Ovsiannikov O.V.	176
Ovsiienko I.V.	32, 34, 43

P

Paineau E.	7
Palchekovskiy O.A.	147
Palchik O.V.	213
Pampuha I.	218
Panasiuk Y.D.	284
Panchenko A.I.	226
Panko A.V.	246, 255

- Paryzhak S. 224, 283
 Pasenko O.O. 316
 Pashchenko A.V. 9, 10
 Pashchenko E.O. 344
 Pashkevich Yu. G. 509
 Pashynska V.A. 153
 Pasmurtseva N. 96
 Passirani C. 78, 224
 Patrylak L.K. 197
 Pavlenko O.L. 109, 238, 278
 Pavliuk M. 519
 Pavlov V.O. 360, 530
 Pavlyshche N.I. 463
 Pavlyuk D.O. 49, 50
 Pazdriy Ya.Ye. 174
 Penuykh B. 439
 Pereira M.F. 458
 Perekos A. 88, 333
 Perepelytsia V.K. 516
 Perepelytsya S.M. 531
 Perepichay M. 312
 Perets Y.S. 43
 Perets Yu.S. 2, 58, 174
 Permyakova N.M. 130
 Pershina K.D. 379
 Pertko O. 82
 Pertko O.P. 126, 197
 Petrenko O.V. 111
 Petrosian L.I. 325
 Petrov E.G. 415, 492
 Petrov V.V. 114
 Petrovska S.S. 380
 Petruniak O. 444
 Petrusha I. 158, 446
 Pham T. 299
 Piatnytskyi D.M. 400
 Pilcevich N. 241
 Pinchuk N. 96
 Pinchuk-Rugal T.M. 109
 Pirro P. 497
 Piryatinski Yu.P. 101
 Plecenik T. 25
 Plevachuk Yu. 170, 500
 Plutenko T.O. 188, 332, 370, 500
 Poderys V. 375
 Podhurska V. 398
 Podshebiakin A.O. 428
 Pogodin A. 84
 Pogodin A.I. 485
 Pogorielov M. 408, 411
 Pokhylko B. 80
 Pokynbroda T.Y. 191
 Polek T. 483
 Polewczyk W. 408, 411
 Polikarpova L.O. 15
 Polishchuk S. 508
 Politanskyi R.L. 381
 Polotskyi D.Yu. 105, 435, 498,
 512, 516
 Polotskyi D.Yu. 498
 Poltoratska T. 96
 Polyakov S.V. 338
 Polynchuk P.Yu. 6
 Pomastowski P. 206, 209, 211
 Ponomar I.A. 73
 Pop M.M. 485
 Popil O.I. 305
 Popilovskyi N. 369
 Popov M.O. 336, 346, 361, 362, 363,
 364, 370, 371, 372
 Popov O. 139
 Popovych A. 98
 Popovych D.I. 144, 351, 507
 Popovych V. 98
 Poroshin V.N. 80, 215
 Porowski S. 446
 Potapenko H. 180
 Potapenko O. 180
 Potomkina Zh.V. 269
 Potupa V.Y. 296
 Povazhny V.A. 340
 Povazhnyi V. 82
 Povazhnyi V.A. 4
 Poverzhuk V. 500
 Poyedinok N.L. 269
 Pozhar V.V. 423
 Pozniak O.R. 318, 319
 Prikhna T.O. 15
 Pritula I. 349
 Prokhorenko D.K. 203
 Prokhorenko S.V. 89
 Prokopchuk M. 453
 Prokopenko S.L. 69
 Prokopenko V.A. 160, 187,
 246, 330
 Prokopiuk V.Yu. 247, 248
 Prozar D. 444
 Prudius S.V. 304
 Pruntseva G.O. 285
 Prybora N.A. 341
 Pryhunova O. 81, 143
 Prylutska S.V. 301

Prylutsky Yu.	218, 221, 230
Pryshchepa O.	206, 209, 211
Prystash M.S.	89
Prysyazhnyuk V.I.	528
Ptashnyk V.	135
Pu Y.	339, 342
Puz'ko O.A.	418
Pužniak R.	481
Pyeshkova V.M.	284, 294
Pylypchuk O.	534
Pylypchuk O.S.	80, 215
Pylypenko A.	235
Pylypko V.G.	54
Pylypov A.I.	501
Pylypova O.	108, 159, 375, 501

R

Rachiy B.I.	16, 113
Radchenko T.M.	503
Rader O.	405
Radio S.V.	202, 355
Rakickas T.	443
Rakytka T.L.	524, 524
Rallev M.	534, 537, 539
Rashydov N.M.	273
Razumiene J.	250
Redko A.V.	4
Redko R.A.	472
Redko S.M.	472
Remezovskiy I.M.	126
Reshetnyak V.	443
Reshetnyk M.	486
Reva V.I.	461
Riabov S.V.	61, 280
Rieznichenko L.S.	80, 246, 293
Ripko O.P.	50
Ritter U.	218, 230, 301
Rizak V.M.	393, 506
Rodik R.V.	226, 267
Rogachova O.	529
Roik N.V.	8
Romanova I.V.	379
Romanovska N.	402
Romantsova O.	194
Romanyuk B.M.	350
Romanyuk V.	532
Romanyuk V.R.	412
Ronkovych A.V.	149, 150
Ropakova I.Yu.	23
Roshchin O.M.	438

Rotomskis R.	375
Rouquier Ph.	457
Rozantsev G.M.	202
Rozenbaum E.V.	273
Rozhdestvenska L.	180
Rozhdestvenska L.M.	213
Rozhdestvenska L.M.	86
Rozhin A.G.	101
Rud A.D.	94, 174, 182
Rudenko E.M.	435, 498, 512, 516
Rudenko E.M.	105, 498
Rudenko V.I.	416
Rudko G.	390, 429
Rudnytska O.V.	270
Rugal A.G.	109
Rumiantseva Y.	518
Rusakov V.F.	481
Ryabchenko S.	483
Ryabtsev S.I.	46, 64
Rybalchenko N.P.	220
Rybalko A.	373

S

Sadova N.M.	20
Sadovyi B.	158, 446
Sadovyi P.	158, 446
Sadowski J.	532
Sahraoui B.	457
Sakhnenko M.D.	155
Saliy Ya. P.	394
Samaryk V.Y.	195, 198, 298
Samchenko K.	96
Samchenko Yu.	96
Samoilov O.M.	23
Samoylov A.V.	466
Sánchez-Barriga J.	405
Sanguinetti S.	258, 388
Satrapinskyy L.	25
Saulnier P.	78, 224
Savchenko B.M.	141
Savchenko D.	333
Savchenko D.O.	344
Savchenko I.	118
Savchenko I.O.	360
Savelyev Yu.V.	136
Savka S.S.	507
Sawicki M.	532
Scheludko V.	356
Scherbatskyi V.	210

- Scherbatskyi V.P. 374
 Schevchenko V. 356
 Schönhense G. 532
 Schuba S. 243
 Schwarz S. 382
 Schweiger L. 152
 Sedyh O.O. 232, 236
 Sembratovych N. 369, 448
 Semenko M.P. 327
 Sementsov Y. 87
 Sementsov Yu. 356
 Sementsov Yu.I. 40, 48, 69
 Semerenko Y. 18
 Seminko V. 106, 110,
 129, 225, 367
 Semjonova A. 205
 Semkiv I.V. 384
 Sencha-Hlevatska K. 87
 Serbeniuk T.B. 15
 Serdiuk I.V. 401
 Serednytski A.S. 351
 Sergeyeva T.A. 282
 Sergiienko R.A. 14, 380
 Serkiz R. 158
 Serozhkin Yu. 521
 Shablykina O.V. 358
 Shafranyosh I.I. 274
 Shafranyosh M.I. 274
 Shalai Ya.R. 239
 Shamaev V.V. 41
 Shandura M. 526
 Shapovalov A. 41
 Shapovalov Yu.O. 45
 Sharanda L.F. 8
 Shcherbak O.V. 261
 Shcherban N.D. 71, 310, 338
 Shcheretskyi O.A. 14
 Shcheretskyi V.O. 14
 Shchetinin M.S. 442
 Shchokotova O.M. 21
 Shelest T. 529
 Shelkovsky V.S. 153
 Sheludko V.I. 53
 Shender I. 84
 Shepa I. 134
 Shepida M.V. 397
 Shevchenko A.B. 496
 Shevchenko O.O. 374
 Shevchenko V. 211
 Shevchenko V.B. 374
 Shevchenko V.V. 347
 Shevchenko Ye.V. 415
 Shevchuk S.M. 121
 Shevtsova T. N. 509
 Shkotova L.V. 296
 Shkurdoda Yu. 25
 Shlapa Y. 483
 Shlykov S.G. 226
 Shmeleva L. 443
 Shokatayeva D. 297
 Shpetnyy I. 25
 Shpotyuk Y. 453, 454, 455
 Shpylka D.O. 32, 34
 Shpylovyy P.B. 494
 Shtablavyi I. 369
 Shtapenko E.Ph. 162
 Shuaibov O.K. 47
 Shulga S.M. 233
 Shulyma S.I. 308, 337, 418
 421, 441
 Shulzhenko D.M. 196, 216
 Shumilin S.E. 45
 Shuryhin F.M. 60
 Shut M.I. 34
 Shvachko N.K. 308, 337, 421, 441
 Shvalagin V.V. 472
 Shvernyk V.R. 361
 Shvets O.V. 131, 187, 255,
 310, 311, 338
 Shvets U. 25
 Shylo S.I. 465, 466
 Shymanskyi I.O. 256
 Shymchyshyn O.Y. 133
 Sichkar T.G. 34
 Siharova N.V. 48
 Sinelnikov S.I. 61
 Šipková A. 75
 Siraya O.A. 105
 Siromolot A.A. 256
 Skabara P. 424, 425
 Skakunova O.S. 503
 Skaterna T.D. 301
 Skiba M. 177, 178, 187
 Skopińska-Wisniewska J. 252
 Skorenkyy Yu. 55, 504
 Skorobohaty T.V. 315
 Skoryk M.A. 94, 174, 182, 508
 Skosar V.Yu. 85
 Skrypka A.V. 341
 Skryshevsky V. 108, 159, 375
 Skwarek E. 27
 Skyba Y. 177, 178, 187

Slavin A.N.	488	Stasiv V.	140
Slobodianiuk D.V.	484	Stefaniuk I.	98
Slobodnyj V.A.	406	Stelmakh S.	96, 97, 116
Slobodyanik M.	111	Stepanenko Ye.Yu.	272
Slobodynyk M.S.	137, 179	Stepanian S.G.	153
Slobodzyan D.	173, 453, 454, 455	Stepanov O.	172
Slyvka A.A.	383	Stepanova I.I.	155
Smachylo Yu.	469	Stepanyuk A.N.	335
Smalyuk A.	505	Sternik D.	118
Smarsly B.	206, 211	Stetsenko D.O.	39, 80, 215
Smirnov A.	18	Stetsiuk A.V.	531
Smirnov S.N.	45	Stetsko A.E.	475
Smokal V.O.	449	Stetsyna A.	469
Smolianets R.	18	Stolbovyi V.O.	401
Smolienko N.P.	236	Stoll S.	186
Smolyak S.S.	368	Stolyarchuk A.I.	98, 99, 477
Smyk N.I.	234	Stratilat D.P.	426, 432
Sobolevskyi M.S.	466	Strativnov E.V.	157, 163
Sofronov D.	349	Strelchuk V.V.	158, 350, 440, 446
Sokoliuk D.	235	Strilchuk O.	390
Soldatkin A.P.	80	Strizhak P.E.	132, 300
Soldatkin O.O.	243, 284, 292, 294, 466	Strutynska N.Yu.	44, 62, 111, 203
Solodukha H.A.	358, 360, 530	Studenyak Ya.	84
Solomenko A.G.	335	Studzinsky S.L.	358, 360, 530
Solopan S.	483	Stukanova D.	146
Soloviev E.	375, 521	Stupin Yu.D.	332, 500
Soloviev S.O.	126, 131	Styopkin V.I.	80, 215, 416
Solovyov M.V.	448	Suchocki A.	124, 140, 210
Solyanik G.	525	Sukhatskiy Y.V.	397
Song Chunrui.	10	Sukhenko I.V.	368
Soroka A.P.	421	Sukhoveev O.V.	233
Sorokin O.V.	23	Sukhovia M.I.	274
Sorror S.	123	Sula M.P.	199
Sosnovska M.O.	531	Suprun A.	443
Sova N.V.	141	Sushko M. Ya.	107
Spallek D.	208	Sutkovy P.G.	494
Springholz G.	63, 76, 405	Suvorova Y.	312
Sribna V.	204, 241	Suyindykova G.S.	297, 299
Stadnik V.	518	Svavil'nyi M.Ye.	105, 435, 498, 512
Stadulis J.	181, 186	Švec P.	170
Stakhira P.	424, 425, 442	Švec P. Sr.	500
Stakhira P.Y.	431	Svechnikova O.S.	480
Starinets S.	541	Sverdun V.B.	15
Starokadomsky D.	486	Świec P.	200
Starostenko O.M.	196, 216	Sych O.	88, 96, 97, 116
Staryk S.P.	340	Sydorchuk V.	27, 28
Starykov H.O.	422	Synytsia A.	88, 97, 116
Stasiuk A.V.	195, 198	Syrovatko Yu.V.	162
Stasiuk O.	51, 531	Sytnyk I.O.	5, 286
Stasiuk O.O.	30, 31, 42	Syzonenko O.M.	89
Stasiuk Yu.	84	Szalaŭ U.	97, 116

Szewczuk-Karpisz K.	293
Szewczyk D.	194
Szymczykiwicz E.	135

T

Tabachnikova E.D.	45
Takagaki Y.	208
Tamarkina Yu.V.	4
Taran A.V.	401, 408, 411
Taranyik G.	228
Taras R.S.	195, 298, 452
Tarenkov V.	41
Tartachnik V.P.	426, 432
Tatarchuk D.D.	10
Tataryn N.	532
Terebilenko K.	137
Terebilenko K.V.	124, 179, 348
Terentieva Yu.G.	37, 272
Tereshkov M.V.	352
Terets A.D.	357, 490
Terets M.I.	40, 48
Teslenko V.I.	260
Teslia R.	502
Teterya M.	469
Tigunova O.O.	233
Tikhonov E.A.	428
Tikhonovsky M.A.	45
Timoshevskii A.N.	510
Titenko A.	333
Titenko O.	333
Titov I. M.	37, 461
Tiutiunnyk A.	56
Tkach N.V.	58
Tkachenko A.A.	479
Tkachenko A.S.	247, 248
Tkachenko I.M.	347
Tkachenko T.	92
Tkachenko T.V.	4, 340
Tkachenko V.	451
Tkachuk T.	166
Tolochyn O.	152
Tomashyk V.M.	387
Tomiesko O.	13
Tomila T.	97, 116
Tomina A.-M.	305
Tomina A.-M.	46
Topchylo A.	159
Toporova O.K.	237
Toroń B.	235
Torpakov A.S.	89

Tovstenko-Zabelin M.S.	67
Tovstolytkin A.	483
Trachevskiy V.	333
Trofymchuk I.M.	8
Trostianchyn A.M.	354
Trots V.V.	66
Trybel A.	92
Trypolskyi A.I.	132, 300
Tsaryuk D.V.	94
Tshehnyi V.	70
Tsekhmister Ya.	408, 411
Tsizh B.	419
Tsybrii Z.F.	350, 435, 440
Tsybrivskiy V.V.	397
Tsyhanovych O.A.	246, 330
Tsybalyuk O.	375
Tsybalyuk O.V.	267
Tulupenko V.	56
Tunyk S.M.	492
Turchak S.	181, 186
Turko B.	158, 164, 446
Turkov O.V.	2, 58
Turowski B.	405
Turutanov O.G.	404
Tuziak O.Ya.	309
Tverdokhle N.	230
Tverdyi D.O.	253
Tymkiv Y.V.	173
Tymoshenko O.I.	401
Tymoshyk A.A.	280
Tyshyk Yu.	398

U

Ubizskii S.	518
Unuchko S.V.	240
Usenko M.O.	237
Ushii L.I.	488
Ustinov A.	508

V

V'yunov O.I.	332, 370, 500
Vainberg V.V.	80, 215, 475
Vakula V.L.	479
Vakuliuk P.	206, 209, 211
Vakyla Y.A.	112
Valihura K.V.	154
Vareniuk I.	218
Varlan K.	312
Varvarenko S. M.	298

- Varvarenko S.M. 195, 198, 298
 Varvarin M. 519
 Varykhalov A. 405
 Vashchenko O.V. 345
 Vashchynskyi V.M. 100
 Vasil'yev V. 158, 164
 Vasin A. 429
 Vassilyeva O.Yu. 111
 Vasylychshyn I. 165
 Vasylechko L. 181, 186, 192, 204, 518
 Vasyliiev T. 452
 Vasyliuk O.M. 62
 Vasyliiv B.D. 318, 319, 320, 321, 322,
 323, 324
 Vasylyuk S.V. 249
 Vavrukh V.I. 318, 319, 320, 321, 322,
 323, 324
 Vazhnenko R. 139
 Vedel D. 51, 531
 Vedel D.V. 30, 42
 Veiksina S. 408, 411
 Veklich A. 189
 Veliky M.M. 256
 Venhryn Yu.I. 351
 Venikov V.O. 121
 Verba R. V. 484, 488, 497
 Verbinska G.M. 366
 Verbitsky A.B. 101
 Verbovytskyi Yu.V. 300
 Vergun L.Yu. 480
 Verkhovliuk A.M. 14
 Vichi S. 388
 Vidal Barrero J.F. 154
 Viletska Yu.M. 270
 Villanueva Perales A.L. 154
 Vinnikov N. 194
 Vira V.V. 318, 319, 320, 321, 322,
 323, 324
 Virych P.A. 222, 244
 Vistak M.V. 381
 Vitusevich S. 125, 392
 Vlasiuk O.M. 531
 Voisin L. 380
 Voitechovic E. 443
 Voitenko O.Y. 330
 Voitovych I.S. 83
 Volobuev V.V. 405
 Voloshyna I.M. 296
 Voloshyna Yu. 82
 Volyniuk D. 424, 425
 Vorobets V.S. 359
 Vorobiov S. 84, 134, 393, 506
 Vorobyova V. 177, 178, 187
 Voropai G.V. 109
 Vorotytskyi P. 96
 Vortman M. 211
 Vovchenko L.L. 2, 34, 43,
 58, 141, 174, 182
 Vovk O. 373
 Voznesenska T. 241
 Voznyak A.V. 103
 Vretik L.O. 67, 428, 430
 Vynnyk A. 454
 Vyshnevskaya Yu.P. 306
 Vyshnevsky S.G. 226
 Vysotskyi P. 63, 76
 Vyunov O.I. 188
- W**
- Wang Q. 497
 Wlazlowska E. 185
 Wodak I. 76, 169, 170, 76
 Wojciechowski T. 405
 Wojtowicz T. 405
 Wosinski T. 532
 Wu Min 40
- Y**
- Yablochkova K.S. 480
 Yakovenko A.V. 197
 Yakovenko O.S. 2, 43, 58,
 174, 182
 Yakymovych A. 76, 169, 170, 500
 Yanchevskii O.Z. 188, 332, 370, 500
 Yang J. 339, 342
 Yanovska E. 118
 Yanushevskaya O.I. 156, 399
 Yaremchuk G. 125
 Yaremchuk I. 38, 424, 469
 Yaremiy I.P. 113
 Yaremkevych A. 534, 536, 537, 539,
 541
 Yaremov P.S. 338
 Yarynka D.V. 282
 Yaschenko O. 210
 Yashchenko O.V. 124
 Yashchuk V.P. 428, 430
 Yastrubchak O. 532
 Yatsiuk M.V. 109
 Yatskiv R. 429

Yatskiv R. 429
 Yavorska L.O. 394
 Yavorskyi R. S. 394
 Yefimova S. 23, 106, 110, 129, 225, 232,
 236, 247, 248, 367
 Yelisieiev M.Y. 80, 215
 Yemets A.I. 276
 Yermukhamed D. 297, 299
 Yeshchenko O. 78, 79
 Yeshchenko O.A. 412
 Yesikov K.Y. 305
 Yevdokimova O. 71
 Yevdokymenko V.O. 4, 340
 Yevych Ya. 88
 Yuhkymchuk V. 375
 Yurieva K.A. 490

Z

Zabashta Yu.F. 480
 Zabolotnii Ye.V. 29
 Zabolotnyy I.M. 503
 Zabudsky V.V. 350
 Zaderko A. 159, 297, 450
 Zaderko O. 429
 Zafar H. 458
 Zagorodnii V. 88
 Zagorodnii V.V. 2, 141
 Zagorodniy Yu.O. 368
 Zahornyi M.M. 7
 Zahorodnia S.D. 220, 251
 Zahorulko I. 508
 Zaiats D.O. 2, 43, 58
 Zaichenko A. 17
 Zaichenko O.S. 239
 Zaika S.O. 395
 Zaika V.V. 337, 421, 441
 Zain S. 392
 Zhulai D. 392
 Zaitsev D.V. 249
 Zakarian D. 104
 Zakusylo T. 63, 76
 Zakutevskyy O. 27
 Zaleszczyk W. 405
 Zapukhlyak R.I. 16
 Zarembo A.A. 251
 Zarembo P.Yu. 251
 Zarkov A. 181, 186
 Zatovsky I.V. 160, 187, 246, 255
 Zavaliy I. Yu. 161, 300
 Zavialych D. 259
 Zazhigalov V.O. 29
 Zeng D. 3, 5, 184
 Zhang J. 339, 342
 Zhao X. 243
 Zharka V. 13
 Zheltonozhskaya T.B. 67
 Zhokh O.O. 132
 Zholkovskiy E.K. 307
 Zholobak N.M. 256
 Zhou R. 339
 Zhuchenko Z. 208
 Zhuchenko Z.Y. 452
 Zhulai D. 125, 392
 Zhuravkov O.V. 2
 Zhuravskiy S.V. 48
 Zhydachevskyy Ya. 518
 Zhydachevskaya H. 518
 Zhydachevskyy Ya. 124, 140, 505
 Zhydenko I. 167, 168
 Zhylytsya S.V. 122
 Zhytnyk D.O. 336, 346, 361, 362, 363,
 364, 365
 Zhytskyi A.K. 22
 Zikrata O.V. 126, 128, 131
 Zinoune J-B. 78
 Zinoviev P. 18
 Zobnina V.G. 153
 Zoryansky V. 18
 Zozulia V.O. 179
 Zraichenko O.V. 404
 Zueva N.O. 368

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Structural, electronic and optical properties of CdLiF_3 and CdLiCl_3 halide perovskites using first-principles calculation

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The structural, electronic, and optical characteristics of CdLiF_3 and CdLiCl_3 halide perovskites were calculated using first-principles calculations based on density functional theory (DFT) employing the generalized gradient approximation (GGA) approach [1,2]. The structural parameters, comprising the lattice constants (a), bulk modulus (B), and its pressure derivative (B'), were computed for the examined compounds. The optimal lattice parameters were $a=b=c= 3.699 \text{ \AA}$ for CdLiF_3 and $a=b=c= 4.607 \text{ \AA}$ for CdLiCl_3 . The electronic band structures and their associated total and partial density of states diagrams were also estimated. The compound CdLiF_3 is a semiconductor with a bandgap of 1.96 eV, whereas CdLiCl_3 is a semimetal conductor. The spectra of the frequency-dependent complex dielectric function, absorption coefficient, refractive index, extinction coefficient, reflectivity, and electron energy loss function were computed and analyzed.

Keywords: halide perovskites; First-principles calculation; Structural parameters; Electronic structure; Optical functions.

1. Clark S. J., Segall M. D., Pickard C. J., Hasnip P. J., Probert M. J., Refson K., Payne M. C. First principles methods using CASTEP// *Zeitschrift fuer Kristallographie*. -2005.-**220**.-P. 567-570

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