

Seán R. Kavanagh

PhD Researcher

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Flash Summary

- Published over 21 peer-reviewed papers over 3 years in top-tier journals (Nature Photonics, Nature Communications, npj Comp Mater, Chemical Science, ACS Energy Letters, Materials Horizons, Matter...), including 9 as first-author and 5 as corresponding author.
- Several papers are the result of MSc / PhD projects I designed and supervised.
- UCL Mathematical & Physical Sciences (MAPS) Faculty Education Award, for Individual Excellence in academic supervision and personal tutoring.
- MRS Graduate Student Awards (Gold 2023, Silver 2022), Materials Today Chemistry Rising Star Award, eMRS Young Researcher Award, 2 eMRS Graduate Student Awards, Ramsay Medal (and Catlow Prize) for Best (Computational) Chemistry PhD student in UCL Chemistry 2022.

Education & Research Experience

2023-10 - Ph.D.: Computational Materials Science (London, UK)

2020-02 Profs David Scanlon (University College London) & Aron Walsh (Imperial College London)
Modelling defects, disorder and bulk properties of solid-state energy materials, primarily solar photovoltaics (incl. non-radiative recombination) but also batteries, thermoelectrics, LEDs/emission (exciton self-trapping), COFs, ferroelectrics, using DFT, GW+BSE and some ML.

- Designed & supervised >20 MSc & PhD projects, yielding papers in *Matter*, *npj Comp Mater*, *ACS Energy Lett...* alongside multiple prizes for excellent supervision.
- Month-long research stays (Max Planck and JSPS Awards; €1k & £3k) with Profs. Freysoldt (Germany) & Kumagai (Japan); paper in *Faraday Discussion*, 2 in submission.
- Lead tester of VASP (most widely-used computational materials science code worldwide) for Archer2 (UK National Supercomputer), and lead research consultant for procurement of UCL HPC & GPU upgrades 2021/2022 (>£1 million).
- Archer2 Pioneer Project Grant lead author; notional value £110k.
- Peer reviewer for *J. Am. Chem. Soc. (JACS)*, *Appl. Phys. Lett. (APL)*, *Matter*, *Phys. Rev. Appl. (PRA)*, *J. Phys. Chem. Lett. (JPCL)*, *Phys. Rev. X (PRX)*, *Energy*, *Phys. Rev. Mater. (PRM)*, *ACS Nano Lett.*, *Comp. Phys. Comm.*, *IOP Model. Simul. Mat. Sci. Eng.*, *JECR...*
- Average 3.5 talks at each MRS Spring/Fall conference since Fall 2020 (1st year PhD).
- Session chair for MRS Fall CH02 (2021) and EN02 (2022) Symposia.
- Featured in the Irish Times: [Irish Scientists Shine in Solar Cell Development](#).
- UCL Mathematical and Physical Sciences (MAPS) Faculty Early Career Researcher (ECR) advisory committee member, and ECR awards judging panel.

- UCL Resources for New Chemistry Researchers (Computational Chemistry) Tutor and 'Python for Chemical Modelling' module Graduate Teaching Assistant (GTA) at UCL.
- Developer of computational chemistry tools: [ShakeNBreak](#), [vaspup2.0](#) and [doped](#), co-developer of [sumo](#), [surfaxe](#), [easyunfold](#), [PyTASER](#), [CarrierCapture.jl](#) ...

2018-09 - Research Assistant

2018-05 *NOKIA Bell Labs, Dublin, Ireland*

Research project employing chemical and electrochemical techniques to fabricate microporous, structured surfaces for efficient heat dissipation from 5G devices.

2019-05 - B.A. (Mod): Nanoscience, Physics And Chemistry of Advanced Materials

2015-09 *Trinity College Dublin – Ireland*

Graduated top-of-the-class (margin >10%), Gold Medal, with First Class Honours (88%).

- Henderson-Lloyd prize for the highest overall grade in the Class of 2019, in the Schools of Chemistry and Physics at Trinity College Dublin (margin >10%).
- Trinity Employability Award in Partnership with Intel (2018).
- Elected to Foundation Scholarship, the "most prestigious undergraduate award in Ireland" (€100,000 Value)(2017).
- Represented Trinity College Dublin in the Eurachem Analytical Measurement Competition, achieving 2nd place out of 20 (2017).

2015-05 - High School

2009-09 *Castleknock College - Dublin, Ireland*

10th highest performer in the nationwide High School Leaving exams out of 58,000 students; amongst only 7 students to achieve 100% in Chemistry, and 3 for 100% in Maths.

Awards

- UCL Mathematical & Physical Sciences (MAPS) Faculty Education Award, for Individual Excellence in academic supervision and personal tutoring.

Research Excellence Awards

- MRS Gold Graduate Student Award & Future Leader 2023.
- *Materials Today Chemistry* Rising Star Award 2022.
- Materials Research Society (MRS) Future Leader 2022.
- European Materials Research Society (eMRS) Young Researcher Award 2022.
- MRS Graduate Student Award (Silver) 2022.
- Ramsay Medal for Top Chemistry PhD student in UCL & Catlow Prize for Top Computational Chemistry PhD – typically awarded to final year PhDs, both received in my 2nd-last year.
- eMRS Graduate Student Award 2021 (Symposium A) for outstanding research performance in the field of materials for energy applications.
- eMRS Graduate Student Award 2021 (Symposium F) for outstanding research performance in the field of earth-abundant next-generation solar cell materials.

- Shortlisted for the International Conference on Defects in Semiconductors (ICDS) 2021 [Corbett Prize](#) (typically awarded to Associate Professors).
 - In addition, MSc students I've supervised have won the Nyholm (Best Inorganic MSc Project in UCL Chemistry) & Sharp (Best Theoretical) prizes.

Travel Awards & Grants

- UCL-McGill-JSPS Core-to-core research collaboration grant (£3k) to visit Prof. Yu Kumagai in Tohoku University (October – November 2022), to extend our defect structure-searching work.
- Max Planck Travel Award (€1k) for a research stay with Prof. Christoph Freysoldt at Max-Planck-Institut für Eisenforschung (MPIE), Germany (October – November 2022).
- Thomas Young Centre (TYC) Junior Research Fellowship (JRF), 2021 (£1k).
- École Polytechnique Fédérale Lausanne (EPFL) Young Scientist Travel Award 2021.
- Royal Society of Chemistry (RSC) Researcher Development Grant, 2021.
- UCL Mathematical & Physical Sciences Faculty Early Career Researcher Travel Grant (£800).
- Royal Society and UCL Nominee to attend the tri-annual Nobel Chemistry Laureate Meeting in Lindau, Germany, at which I was awarded the Lindau Spirit Fellowship for highly-promising young researchers; given to 4 junior lecturers, 1 postdoc and 1 PhD (me).
- RSC Solid State Chemistry Group Travel Award 2022.

Presentation Prizes & Awards

- Roy Prize for Best Graduate Student Oral Presentation at the RSC 40th Anniversary Solid State Chemistry Group (SSCG) Meeting, 2021 (£250), judged by the invited speakers.
- Best Poster Prize at the RSC International Conference on Materials Chemistry (MC16) – '*Tin & Titanium Vacancy-Ordered Halide Perovskites: Cs₂(Sn/Ti)X₆*'
- Excellent Talk Prize at MRS Fall 2022 – '*Impact of Cation Disorder in ABZ₂ Solar Absorbers*'
- Best Presentation Award at EMRS Spring 2022 – '*Cation disorder engineering in AgBiS₂*'
- Excellent Talk Prize at MRS Fall 2020 – '*Enhanced Optical Absorption via Mixed-Valent Doping of Vacancy-Ordered A₃B₂X₉ Triple Perovskites*'.
- Excellent Talk Prize at SCI Materials for Energy Technology 2021 – '*Rapid Recombination by Cadmium Vacancies in CdTe*'.
- Best Poster at TYC Conference 2020, King's College London – '*Band Alignment of Antimony and Bismuth Silver-Bromide Double Perovskites*'.
- Excellent Poster Prize at RSC Materials Chemistry Poster Symposium 2021 – '*Bandgap Lowering in Lead-Free Cs₂Ag(Sb_xBi_{1-x})Br₆ Double Perovskite Alloys*'.
- Best Poster Prize at UCL Chemistry PhD Poster Session (2021) – '*Hidden spontaneous polarisation in the chalcogenide photovoltaic absorber Sn₂SbS₂I₃*'.

Publications (*h*-index = 11)

* = Corresponding Author

(1) **Kavanagh, S. R.** & Wang, Y. (co-authors); Burgués-Ceballos I.; Walsh, A.; Scanlon D., Konstantatos G. Cation Disorder Engineering Yields AgBiS₂ Nanocrystals with Enhanced Optical Absorption for Efficient Ultrathin Solar Cells. *Nature Photonics* **2022**, 16 (3), 235-241

(March Issue 'Hero' Image, featured on many [news sites](#)) – 61 citations – doi.org/10.1038/s41566-021-00950-4

(2) Huang, Y.; **Kavanagh, S. R.**; Scanlon, D. O.; Walsh, A.; Hoyer, R. L. Z. Perovskite-Inspired Materials for Photovoltaics and beyond — from Design to Devices. *Nanotechnology* **2021**, 32 (13), 132004. (Authored Sections 1, 2 & 6) 98 citations (**most read/cited 2021 article in IOP Nanotechnology**) – doi.org/10.1088/1361-6528/abcf6d

- Spotlighted in *Nature Physics* ([link](#)), before publication.

(3) **Kavanagh, S. R.*** & Mosquera-Lois, I. (co-authors); Walsh, A.; Scanlon, D. O. Identifying the Ground State Structures of Defects in Solids. *npj Computational Materials* **2023** 9(25) – 9 citations – doi.org/10.1038/s41524-023-00973-1

- Spotlighted in *Nature Physics* News & Views (<https://www.nature.com/articles/s41567-023-02049-9>)

(4) **Kavanagh, S. R.*** & Mosquera-Lois, I. (co-authors); Walsh, A.; Scanlon, D. O. ShakeNBreak: Navigating the defect configurational landscape. *Journal of Open Source Software* **2022**, 7(80), 4817 – 6 citations – doi.org/10.21105/joss.04817

(5) **Kavanagh, S. R.** & Huang, Y. (co-authors); ... Unold, T.; Stranks S. D.; Rao, A.; Herz L. M.; Scanlon, D. O.; Walsh, A.; Hoyer. Strong Absorption and Ultrafast Localisation in NaBiS₂ Nanocrystals with Slow Charge-Carrier Recombination. *Nature Communications* **2022** 13 (1), 1-13 – 9 citations – doi.org/10.1038/s41467-022-32669-3

(6) **Kavanagh, S. R.** & Li, Z. (co-authors)... Friend, R. H.; Scanlon, D. O.; Walsh, A.; Hoyer, R. L. Z. Bandgap Lowering in Mixed Alloys of Cs₂Ag(Sb_xBi_{1-x})Br₆ Double Perovskite Thin Films. *Journal of Materials Chemistry A* **2020**, 8 (41), 21780–21788 – 54 citations – doi.org/10.1039/D0TA07145E

(7) **Kavanagh, S. R.**; Walsh, A.; Scanlon, D. O. Rapid Recombination by Cadmium Vacancies in CdTe. *ACS Energy Letters* **2021**, 6 (4), 1392–1398 – 32 citations – doi.org/10.1021/acsenergylett.1c00380

(8) **Kavanagh, S. R.**; Savory, C. N.; Scanlon, D. O.; Walsh, A. Hidden Spontaneous Polarisation in the Chalcogenide Photovoltaic Absorber Sn₂SbS₂I₃. *Materials Horizons* **2021**, 8 (10), 2709-2716 – **Outside Front Cover, October Issue** – 18 citations – doi.org/10.1039/D1MH00764E

(9) **Kavanagh, S. R.***; Savory, C. N.; Liga, S. M.; Konstantatos G.; Scanlon, D. O.; Walsh, A. Frenkel Excitons in Vacancy-ordered Titanium Halide Perovskites (Cs₂TiX₆). *J. Phys. Chem. Lett.* **2022**, 13, 10965–10975 – 12 citations – doi.org/10.1021/acs.jpcclett.2c02436

- (10) **Kavanagh, S. R.***; Scanlon, D. O.; Walsh, A.; Freysoldt, C. Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells. *Faraday Discussions* **2022**, 239, 339-356 – 12 citations – doi.org/10.1039/D2FD00043A
- (11) Krajewska, C.J.; **Kavanagh, S. R.**; Stranks, S. D.; Walsh, A.; Scanlon, D. O.; Palgrave, R.G. Enhanced Visible Light Absorption in Layered Cs₃Bi₂Br₉ through Mixed-Valent Sn(II) / Sn(IV) Doping. *Chemical Science* **2021**, 12 (44), 14686-14699 – **Outside Front Cover, November Issue**, 18 citations – doi.org/10.1039/d1sc03775g
- (12) Mosquera-Lois, I.; **Kavanagh, S. R.*** In Search of Hidden Defects. *Matter* **2021** 4 (8), 2602-2605 – *From an MSc Project I designed & supervised.* – 11 citations – doi.org/10.1016/j.matt.2021.06.003
- (13) Wang, X.; Li, Z.; **Kavanagh, S. R.**; Ganose, A. M.; Walsh, A. Lone Pair Driven Anisotropy in Antimony Chalcogenide Semiconductors. *Physical Chemistry Chemical Physics* **2022**, 24 (12), 7195–7202 – 21 citations – doi.org/10.1039/D1CP05373F
- (14) Jaśkaniec, S.; **Kavanagh, S. R.**; Walsh, A.; Scanlon, D. O.; Nicolosi, V. Solvent Engineered Synthesis of Layered SnO for High-Performance Anodes. *npj 2D Mater. Appl.* **2021**, 5 (1), 1–9 – 11 citations – doi.org/10.1038/s41699-021-00208-1
- (15) Brlec, K.; **Kavanagh, S. R.**; Savory, C. N.; Scanlon, D. O. Understanding the Photocatalytic Activity of La₅Ti₂AgS₅O₇ and La₅Ti₂CuS₅O₇ for Green Hydrogen Production: Computational Insights. *ACS Applied Energy Materials* **2022**, 5 (2), 1992–2001 – 8 citations – doi.org/10.1021/acsaem.1c03534
- (16) Antonelli, T.; ... **Kavanagh, S. R.**; ...; Scanlon, D. O.; King, P. D. C. Orbital-Selective Band Hybridisation at the Charge Density Wave Transition in Monolayer TiTe₂. *npj Quantum Materials* **2022**, 7 (98), 1-10 – doi.org/10.1038/s41535-022-00508-9
- (17) Huang J.; Golomb M. J.; **Kavanagh, S. R.**; Tolborg K.; Ganose A. M.; Walsh A. Band Gap Opening from Displacive instabilities in Layered Covalent-Organic Frameworks. *Journal of Materials Chemistry A* **2022** 10 (25), 13500–13507 – 7 citations – doi.org/10.1039/D2TA02993F
- (18) Wang, X.; Ganose, A. M.; **Kavanagh, S. R.**; Walsh, A. Band Versus Polaron: Charge Transport in Antimony Chalcogenides. *ACS Energy Letters* **2022** 7 (9), 2954–2960 – 3 citations – doi.org/10.1021/acsenergylett.2c01464
- (19) Nicolson, A.; Breternitz, J.; **Kavanagh, S. R.**; Tamm, Y.; Morita, K.; Squires, A.; Tovar, M.; Walsh, A.; Schorr, S.; Scanlon, D. O. Interplay of static and dynamic disorder in the mixed-metal chalcogenide Sn₂SbS₂l₃. *Journal of the American Chemical Society* **2023** 145 (23) 12509-12517 – doi.org/10.1021/jacs.2c13336

- (20) Cen, J.; Zhu, B.; **Kavanagh, S. R.**; Squires, A.; Scanlon, D. O. Intrinsic Defect Chemistry of High-Voltage $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ (LMNO) Spinel Cathode. *Journal of Materials Chemistry A* **2023** – doi.org/10.1039/D3TA00532A
- (21) Nicolson, A.; **Kavanagh, S. R.**; Savory, C. N.; Watson, G. W.; Scanlon, D. O. Cu_2SiSe_3 as a promising solar absorber: harnessing cation dissimilarity to avoid killer antisites. *Journal of Materials Chemistry A* **2023** – doi.org/10.1039/D3TA02429F
- (22) Wang, X.; **Kavanagh, S. R.**; Walsh, A.; Scanlon, D. O. Four-electron Negative-U Vacancy Defects in Antimony Selenide. Under review at *Physical Review Letters* (doi.org/10.48550/arXiv.2302.04901)
- (23) Kumagai, O.; **Kavanagh, S. R.**; Tsunoda, N.; Walsh, A.; Scanlon, D. O.; Oba, F. Alkali Mono-Pnictides: Potential High-efficiency Photovoltaic Materials. Under review at *PRX Energy*.
- (24) Jagadish, K... **Kavanagh, S. R.**... Gasparini, N; Dubal, D; Rondiya, S. Interface Characterization Tools for Copper-based Quaternary Chalcogenides: Review and Prospects. *In Submission*.
- (25) Mosquera-Lois, I. **Kavanagh, S. R.**; Klarbring, J; Tolborg, K; Walsh, A. Imperfections are not OK: Free Energy of Point Defects in Crystals. Under review at *Chemical Society Reviews* (Invited Review).
- (26) **Kavanagh, S. R.** & Liga, S. M. (co-authors); Walsh, A.; Scanlon, D. O.; Konstantatos G. Environmentally-friendly mixed titanium/tin (IV) based vacancy-ordered double perovskites. Under Review at *J. Phys. Chem. C*. (Special Issue on physicochemical properties of perovskites).
- (27) **Kavanagh, S. R.***; Kumagai, O.; Scanlon, D. O.; Walsh, A. High-Throughput Study of Symmetry-Breaking at Oxygen Vacancies in Oxides. *In Submission*.
- (28) Don, C. H; Smiles, M. J.; **Kavanagh, S. R.**; Shalvey, T.; Scanlon, D. O.; Veal, T. Band gap and band alignment trends of antimony sulfur/selenide ($\text{Sb}_2(\text{S/Se})_3$) solar cells. *In Submission*.
- (29) Zhu, B.; **Kavanagh, S. R.**; Scanlon, D. O.; easyunfold: A Python package for unfolding electronic band structures. *Under review at Journal of Open Source Software (JOSS)*.
- (30) **Kavanagh, S. R.**; Scanlon, D. O.; Walsh, A.; doped: Calculating point defects in solids. *In submission to Journal of Open Source Software (JOSS)*.

Conference Talks & Posters

See YouTube channel for recorded talks.

1st Year PhD:

'Band Alignment of Antimony and Bismuth Silver-Bromide Double Perovskites' Poster @ NanoGe Online Conference: Beyond Lead Halide Perovskites; TYC Conference 2020, King's College London (**Best Poster Prize**); Talk @ NanoGe ComPer 2020

'Bandgap Lowering in Lead-Free $\text{Cs}_2\text{Ag}(\text{Sb}_x\text{Bi}_{1-x})\text{Br}_6$ Double Perovskite Alloys' Talk@ RSC Solid-State Chemistry ECR Conference; NanoGe Fall 2020 Poster @ NanoGe HOPV 2020; (Flash Talk) MRS Fall 2020; RSC Materials Chemistry Poster Symposium (**Excellent Poster Prize**)

'Enhanced Optical Absorption via Mixed-Valent Doping of Vacancy-Ordered $\text{A}_3\text{B}_2\text{X}_9$ Triple Perovskites' Talk @ MRS Fall 2020 (**Excellent Talk Prize**); NanoGe Fall 2020; MRS Spring 2021; (Invited Talk) @ Morgan Research Group, University of Bath; (**Invited Talk**) Centre for Plastic Electronics (CPE) Perovskite Symposium 2021; RSC SSCG 2021 (**Roy Prize for Best Oral Presentation**), ACS Fall 2021

'Solvent Engineered Synthesis of Layered SnO Nanoparticles for High-Performance Anodes' (Flash Talk) @ MRS Fall 2020

2nd Year PhD:

'UCL Chemistry & Light Highlight Seminar: Modelling Excited Molecules and Materials' (**Invited Talk**) Representing the 30-person Scanlon Research Group, alongside 3 other speakers (all Professors).

'Rapid Recombination by Cadmium Vacancies in CdTe ' Talk @ MRS Spring 2021; NanoGe HOPV 2021, RSC ECR 2021; ACS Fall 2021; eMRS Fall 2021 (**Graduate Student Award**); ICDS31; SCI Materials for Energy Tech (**Excellent Talk Prize**); MRS Fall 2021

'Hidden spontaneous polarisation in the chalcogenide photovoltaic absorber $\text{Sn}_2\text{SbS}_2\text{I}_3$ ' Talk @ MRS Spring 2021; ACS Fall 2021; eMRS Fall 2021 (**Graduate Student Award**); NanoGe HOPV 2021 Poster (**UCL Chemistry Best Poster Prize**); MRS Fall 2021

'Impact of Defect Dynamics on Device Performance: Case Study in CdTe ' (**Invited Talk**) @ Dept. of Computational Materials Design at Max-Planck-Institut für Eisenforschung (MPIE; 2021)

3rd Year PhD:

'Efficient Ultrathin AgBiS_2 Solar Cells via Cation Disorder Engineering' Talk @ IOP & SuperSolar Advances in Photovoltaics 2022 (Sole student speaker), MRS Spring 2022 (**Graduate Student Award**); EPFL SeeFuturePV (**Young Scientist Travel Award**); eMRS Spring 2022 (**Best Presentation Award**), (**Invited Talk**) @ UCL Materials for the Future Mini-Symposium 2022

'Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells' (**Invited Talk**) @ Colorado School of Mines, MRS Spring 2022, RSC Faraday Discussions, eMRS Spring 2022, ETH Zürich Defects in Solids Workshop 2022

'Revealing excitonic behaviour in vacancy-ordered titanium perovskites (Cs_2TiX_6)' Talk @ eMRS Spring 2022 (**Young Researcher Award**), MRS Fall 2022, Poster @ EPFL SeeFuturePV (**Young Scientist Travel Award**), APS March 2023

'Impact of Cation Disorder in ABZ_2 Solar Absorbers' Talk @ MRS Fall 2022 (**Excellent Talk Prize**), MRS Spring 2023, **Invited Talk** @ CDT-ACM Christmas Symposium 2022

'Identifying Ground State Structures of Defects in Solids' Talk @ MRS Fall 2022, Tohoku University 2022, Yokohama University 2022, UCL-JSPS Core-to-Core Biannual Conference 2022, GRC Defects in Semiconductors 2022, APS March 2023

4th Year PhD:

'Impact of Intrinsic & Extrinsic Defects on Optoelectronic Properties in Selenium' Talk @ MRS Spring 2023, RenewPV Workshop (Tallinn, Estonia)

'Symmetry-Breaking and Reconstruction at Point Defects in Perovskites' Talk @ MRS Spring 2023

'Tin & Titanium Vacancy-Ordered Halide Perovskites: $\text{Cs}_2(\text{Sn/Ti})\text{X}_6$ ' **Invited Talk** @ MRS Spring 2023, Poster @ RSC International Conference on Materials Chemistry (MC16) (**Best Poster Prize**)

'Symmetry-Breaking and Reconstruction at Point Defects in Solids' **Invited Talk** @ Summer of Chemical Theory @ WashU 2023

'Performance Boosters to Efficiency Killers; From bulk disorder to isolated defects' Talk @ MRS Spring 2023 (**Gold Graduate Student Award**), RSC International Conference on Materials Chemistry (MC16)

'Shining a light on the future: supercomputers and AI in solar cell research' Invited Outreach Talk @ [Pint of Science Festival 2023](#)

Referees

Prof David Scanlon, Chair of Computational Materials Design, UCL. (d.scanlon@ucl.ac.uk)

Prof Aron Walsh, Chair of Materials Design, Imperial College London. (a.walsh@imperial.ac.uk)

Dr Christoph Freysoldt, Defect Chemistry and Spectroscopy Group, Max-Planck-Institut für Eisenforschung GmbH. (freysoldt@mpie.de)

Prof Yu Kumagai, Professor in Multi-Functional Materials Science, Institute for Materials Research, Tohoku University. (yu.kumagai.b1@tohoku.ac.jp)

Prof Robert Hoyer, Associate Professor of Inorganic Chemistry & Royal Academy of Engineering Research Fellow, University of Oxford. (robert.hoyer@chem.ox.ac.uk)

Dr. Sinéad Griffin, Staff Scientist, Materials Science Division and Molecular Foundry, Berkeley Lab (sgriffin@lbl.gov)