**Jayanthi Kumar**

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**QUALIFICATIONS SUMMARY**

* Research Scientist with eleven years of experimental research experience at the intersection of solid state science and materials science
* Strong organizational skills and experience in managing & executing research projects both independently and within interdisciplinary research teams
* Exhibit excellent problem solving skills, project management, writing, training and interpersonal skills
* Worked on projects for Department of Energy (DOE) and Critical Materials Institute since 2019

**TECHNICAL SKILLS AND EXPERTISE**

* **Synthesis:** Wet chemical, hydrothermal and high temperature solid state synthesis
* **Material characterization**: *Structure analysis* (PXRD, FTIR, Raman, DSC, TGA, AAS, ICP OES, ICP MS, SEM/EDS), *Electrochemical methods* (CV, EIS, battery testing protocols), and *Calorimetry* (room temperature, and high-temperature oxide melt solution calorimetry).
* **Structural studies:** Rietveld Refinement (GSAS, Full Proof), Free Objects for Crystallography, Ab Initio Structure Calculation, Difference Fourier Techniques, DIFFaX Simulations, Lab View, Origin
* Proficient at using Microsoft office (Word, Excel, PowerPoint, etc)

**EDUCATION**

**Ph.D. in Materials Chemistry**, Central College, [Bangalore University](https://bangaloreuniversity.ac.in/), Bangalore, India 2011-2017

**Master of Science (Analytical Chemistry)**, [St. Joseph’s College](https://www.sjc.ac.in/), Bangalore, India 2009-2011

**Bachelors of Science** **(Chemistry)***,* [St. Joseph’s College](https://www.sjc.ac.in/), Bangalore, India 2006-2009

**RESEARCH EXPERIENCE**

**Oak Ridge National Laboratory, Oak Ridge,** **TN, *Postdoctoral Research Associate*** March 2022-Present

* ***Project:*** Direct Lithium Extractionfrom the Geothermal Brine, Clay Minerals and Recycled Batteries
* ***Actions***: Designed novel sorbent materials for direct lithium extraction from geothermal brine

Demonstrated circular economy in Li extraction process by lithiation, delithiation and relithiation

* ***Patent was filed. Worked closely with industrial partners Rio Tinto, and Lithos, met all the deadlines. Hands-on experience with PXRD, FTIR, TGA, SEM/EDS, ICP OES***

**Arizona State University, Tempe, AZ, *Postdoctoral Research Associate*** Feb 2020- March 2022

* ***Project 1***: Entropy stabilization effects and ion migration in 3D hollow halide perovskites
* ***Actions*:** Performed detailed thermochemical studies on a recently discovered new family of 3D hollow halide perovskites which are promising semiconductors for next generation

Thermodynamic measurements were crucial to understanding the significant role of configurational entropy, in stabilizing these hollow perovskites

* ***Conceptualized the idea and initiated collaboration with the renounced scientists in the perovskites field. Tedious calorimetry measurements were conducted to establish the link between entropy and stability***
* ***Project* 2:** Calorimetry Measurements on Sodium and Lithium-ion Battery Materials
* ***Actions*:** Illustrated the role of both thermodynamic and kinetic factors in phase stability of batteries

Thermodynamic driving force behind the phase stability and phase transformation in battery materials

***Comprehended fabrication of coin cell and battery testing protocols***

* ***Project 3*:** Cryogenic Heat Capacity Measurements and Thermodynamic Analysis of Lithium Aluminum LDHs with Intercalated Chloride
* ***Actions***: Conducted calorimetry measurements and heat capacity measurements

Combined enthalpy, and entropy to arrive at the free energy which is directly proportional to the stability of the LDHs

* ***Detailed understanding of LDH structure, role of the water in stabilizing the structure, and importance of calorimetry which sheds light on the stability of LDHs.***
* Other works involving thermodynamic studies on silicon oxy carbides, rare earth phosphates, nitrides, metal-organic frameworks, metal-organic coordination polymers, and glasses were accomplished
* Participated in DOE grant writing with Prof. Navrotsky and the proposal was accepted in 2021

**University of California, Davis, CA, *Postdoctoral Research Associate*** Feb 2019- Jan 2020

* ***Project 1***: Energetics of the Local Environment of Structure Directing Agents Influence Zeolite Synthesis
* ***Actions***: Emphasized the role of thermodynamics in the crystallization

Evaluated the interplay of thermodynamic and kinetic control in zeolite synthesis

* ***Collaborated with Chevron Energy Technology Corporation, hands-on experiences with room temperature calorimeter***

**Indian Institute of Science (IISc), Bangalore, India**, ***Research Associate*** Jan 2018- Jan 2019

* ***Project 1***: Cation Exchange in Anionic Clay
* ***Actions***: Validated chelated metal ion in the galleries of the EDTA intercalated LDH can be replaced by other transition metal ions, depending on the position of the ion in the Irving –Williams series Demonstrated how functionalization can extend the range and versatility of the host-guest chemistry in inorganic layered solids
* ***Synthesis and cation exchange in LDH was challenging, hands on experience using SEM/EDS and Raman***

**Bangalore University, Bangalore India**, ***Graduate student*** Aug 2013-Dec 2017

* ***Project 1***: Synthesis, Structure Characterization of Cation-Ordered Layered Double Hydroxides
* ***Actions:* Synthesized highly crystalline LDHs by exploring wide matrix of precipitation conditions**

**Illustrated the role of the intercalated anion in structure selection of the LDHs**

**Strategically synthesized cation-ordered LDHs with supercell reflections**

**Attempted Rietveld refinement for the cation ordered LDHs**

* ***Provided direct evidence for cation ordering by PXRD, introduced ‘tranlationengleiche’ group-subgroups relationship to reconcile the large mass of PXRD data of LDHs, hands-on experience with PXRD, FTIR, TGA, AAS, Flame Photometry, Ion Chromatography***
* ***Project 2*: Investigated the origin of distortion that arises in the coordination polyhedron in LDHs using DFT Calculations**
* ***Actions:* Investigated Peierls-type distortion and Jahn Teller distortion in LDHs**

**Performed electronic structure calculation to predict the distortion**

**Employed correlation diagrams and the Tanabe-Sugano like diagram to understand understanding of the electronic structure of inorganic compounds exhibiting color**

* ***Conceptualized the idea and initiated collaboration with a computation chemist, adapted and learnt analyzing DFT results***

**PUBLICATIONS**

* **K. Jayanthi**, P. V. Kamath, ‘Observation of Cation Ordering and Anion-Mediated Structure Selection Among the Layered Double Hydroxides of Cu(II) and Cr(III)’ ***Dalton Trans*actions**, 2013, 42, 13220-13230.
* S. Radha, **K. Jayanthi**, J. Breu, P. V. Kamath, ‘Relative Humidity-Induced Reversible Hydration of Sulfate Intercalated Layered Double Hydroxides’ ***Clays and Clay Minerals***, 2014, 62, 53-61.
* **K. Jayanthi**, S. Nagendran, P. V. Kamath, ‘Layered Double Hydroxides: Proposal of a One-Layer Cation-Ordered Structure Model of Monoclinic Symmetry’ ***Inorganic Chemistry***, 2015, 54, 8388-8395.
* **K. Jayanthi**, P. V. Kamath, ‘A Crystal Chemical Approach to a Cation-Ordered Structure Model for Carbonate-Intercalated Layered Double Hydroxides’ ***Crystal Growth and Design***, 2016, 16, 4450-4456.
* **K. Jayanthi**, P. V. Kamath, G. Periyasamy, ‘Electronic Structure Calculations of Cation-Ordered II-III Layered Double Hydroxides: Origin of the Distortion of the Metal Coordination Symmetry’ ***European Journal of Inorganic Chem*istry**, 2017, 2017, 3675-3682.
* G. Jagannath, B. Eraiah, G. Anuraag, F. Hugo, B. Daniela, **K. Jayanthi**, K. Katturi, S.  V. Rao, F. José, A. Kalyandurg, and Amarnath R. Allu ‘Structural and Femtosecond Third-Order Nonlinear Optical Properties of Sodium Borate Oxide Glasses: Effect of Antimony’ ***Journal of Physical Chemistry*** C, 2019, 123, 9, 5591-5602.
* G. Jagannath, B. Eraiah, **K. Jayanthi**, S. R.Keshri, Sudipta Som, G, Vinitha, A. G. Pramod, K. N. Krishnakanth, G. Devarjulu, S. Venugopal Roa, K. Annapurna, Subrata Das, and Amarnath R. Allu ‘Influence of gold nanoparticles on the nonlinear optical and photoluminescence properties of Eu2O3 doped alkali borate glasses’ ***Physical Chemistry Chemical Physics***, 2020, 22, 2019-2032.
* P. Ranjith, S. Sreevalsa, J. Tyagi, **K. Jayanthi**, G. Jagannath, P. Patra, S. Ahmad, K. Annapurna, Amarnath R. Allu, and Subrata Das ‘Elucidating the Structure and Optimizing the Photoluminescence Properties of Sr2-*x*Al3O6F: Eu*x* oxyfluorides for Cool White LEDs’ ***Journal of Alloys and Compounds***, 2020, 826, 154015.
* **K. Jayanthi**, K. F .U Rahman, P. V. Kamath, G. Periyasamy ‘Electronic Transitions in Layered Hydroxides: Consequences of Trigonal Distortion of Octahedral Symmetry’ ***Spectrochim Acta A Molecular and Biomolecular Spectroscopy***,2020, 233, 118192
* S. I. Zones, **K. Jayanthi**, J. Pascual, D. Xie, A. Navrotsky, ‘Energetics of the Local Environment of Structure Directing Agents Influence Zeolite Synthesis’ ***Chemistry of Materials***, 2021, 33, 2126
* P. Ranjith, S. Sreevalsa, Pritha Patra, Sudipta Som, Ammu Menon, **K. Jayanthi**, K. Annapurna, N. M. Anoop Krishnan, Amarnath R. Allu ‘Realizing cool and warm white-LEDs based on color tuneable (Sr, Ba)2Al3O6F: Eu2+ phosphors obtained via a microwave-assisted diffusion medium’ ***Physical Chemistry Chemical Physics***, 2021,**23**, 15245.
* S. Singh, P. Kumar Jha, M. Avdeev, W.L. Zhang, K. **Jayanthi**, A. Navrotsky, H. N. Alshareef, and P. Barpanda ‘Marinite Li2Ni(SO4)2 as a New Member of Bisulfate Family of High-Voltage Lithium Battery Cathodes’ ***Chemistry of Materials***, 2021, 33, 15, 6108.
* T. Subramani, A. Voskanyan, **K Jayanthi**, M. Abramchuk, A. Navrotsky, ‘A Comparison of Order-Disorder in Several Families of Cubic Oxides’ ***Frontiers Chemistry***, 2021, 9:719169.
* S. Yang, **K. Jayanthi**, A. Anderko, R.E. Riman, A. Navrotsky, ‘[Thermochemical Investigation of the Stability and Conversion of Nanocrystalline and High-Temperature Phases in Sodium Neodymium Fluorides](https://pubs.acs.org/doi/abs/10.1021/acs.chemmater.1c02829)’ ***Chemistry of Materials***, 2021, 33, 24, 9571.
* **K. Jayanthi**, G Neilsen, P.F. Rosen, C. I. Anderson, M. S. Dickson,B. F. Woodfield, M. P. Paranthaman, A. Navrotsky, ‘Cryogenic Heat Capacity Measurements and Thermodynamic Analysis of Lithium Aluminum Layered Double Hydroxides (LDHs) with Intercalated Chloride’, ***American Mineralogist****,*2022, 107 (4), 709.
* I. Mandal, S. Chakraborty, **K. Jayanthi**, M. Ghosh, K. K. Dey, K. Annapurna, J. Mukhopadhyay, A. D. Sharma, A. R. Allu, ‘Role of Sodium-ion Dynamics and Characteristic Length Scales in Ion-Conductivity in Aluminophosphate Glass Containing Na2SO4’ ***Journal of Physical Chemistry C***, 2022, 126, 6, 3276.
* P. Barman, D. Dwibedi, **K. Jayanthi**, S. S. Meena, S. Nagendra, A. Navrotsky, P. Barpanda, ‘Aqueous Spray-Drying Synthesis of Alluaudite Na2+2xFe2-x(SO4)3 Sodium Insertion Material: Studies of Electrochemical Activity, Thermodynamic Stability and Humidity Induced Phase Transition’ ***Journal of Solid State Electrochemistry***, 2022, 26, 1941-1950.
* **K. Jayanthi**, I. Spanopoulos, N. Zibouche, A. A. Voskanyan, E. S. Vasileiadou, M. S. Islam, A. Navrotsky, M. G. Kanatzidis, ‘Entropy stabilization effects and ion migration in 3D “hollow” halide perovskites’ ***Journal of American Society***, 2022, 144, 18, 8223.
* P. Patra, R. Kumar, **K. Jayanthi**, M. Fabian, G. Gupta, S. Khan, S. Chakraborty, S. Das, A. A. Allu, K. Annapurna ‘Ln2Te6O15 (Ln=La, Gd, and Eu) “Anti-Glass” Phases Assisted Lanthanum-Tellurite Transparent Glass-Ceramics: Eu3+ Emission and Local Site Symmetry Analysis’, ***Inorganic Chemistry***, 2022,61, 27, 10342-10358.
* S. Singh, A. Neveu, **K. Jayanthi**, T. Das, S. Chakraborty*,* A. Navrotsky, V. Pralong, P Barpanda, Facile Synthesis and Phase Stability of Cu-based Na2Cu(SO4)2.xH2O (x = 0-2) Sulfate Minerals as Conversion type Battery Electrodes*,* ***Dalton Transactions***, 2022, 51, 11169-11179.
* L. D. Gibson, **K. Jayanthi**, S. Yang, N. Thiele, L. M. Anovitz, R. L. Sacci, A. Navrotsky, V. S. Bryantsev, Characterization of Lanthanum Monazite Surface Chemistry and Crystal Morphology through Density Functional Theory and Experimental Approaches, ***Journal of Physical Chemistry*** C, 2022, 126, 44, 18952-18962.
* K. Jayanthi, A. Chaupatnaik, P. Barpanda, A. Navrotsky, Probing Capacity Trends in MLi2Ti6O14 Lithium-Ion Battery Anodes Using Calorimetric Studies, ***ACS Omega***, 2022, 7, 46, 42482–42488.
* A. Reitz, H. Pazniak, C. Shen, H. K. Singh, K. Jayanthi, N. Kubitza, A. Navrotsky, H. Zhang, U. Wiedwald, C. S. Birkel, ‘Cr3GeN: A Nitride with Orthorhombic Antiperovskite Structure’ ***Chemistry of Materials***, 2022, 34,23,10304-10310.
* A. A. Voskanyan, K. Jayanthi, A. Navrotsky, ‘Vacancy Control in TiNb2O7: Implications for Energy Applications’ ***Chemistry of Materials***, 2022, 34, 23, 10311-10319.
* M. Niu, K. Jayanthi, H. Gao,A. P. Solomon, E. C.O'Quinn, L. Su, Y, Qin, M. E. Toimil-Molars, H. Wang, M. Lang, A. Navrotsky ‘Structural and thermodynamic evolution of an amorphous SiOC ceramic after swift heavy ion irradiation’ ***Acta Materialia***, 2023, 242, 118475.
* P. Barman, P. K. Jha, A. Chaupatnaik, K. Jayanthi, R. Prasada Rao, G. Sai Gautam, S. Franger, A. Navrotsky, P. Barpanda, ‘A New High Voltage Alluaudite Sodium Battery Insertion Material’, ***Materials Today Chemistry***, 2023 (Just accepted).

**AWARDS AND LEADERSHIP**

* Senior Research Fellowship (SRF) recipient from Council of Scientific and Industrial Research (CSIR), Government of India (GOI), 2015-17
* Summer Research Fellowship recipient from University Grant Commission (UGC)-Networking center, School of Chemistry, University of Hyderabad, India for the year 2010
* Session Chair for 10th Annual Oak Ridge Postdoctoral Association Research Symposium (ORPA) 2022
* Organized conferences Department of Science and Technology (DST), Government of India (GOI), Innovation in Science Pursuit for Inspired Research (INSPIRE) Science Camp, under Inspired Internship Scheme 2013-2016
* Secretary of Chemical Society 2010-2011, St. Joseph’s College

**PROFESSIONAL ACTIVITIES**

* Review Editor on the Editorial Board of Catalytic Reactions and Chemistry (specialty section of Frontiers in Chemistry).
* Youth Editorial Board member for Material Plus Journal.
* Actively serving as a referee for journals: Actively serving as a referee for journals:

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| Nature Communications | Inorganic Chemistry |
| Journal of American Ceramic Society | Solid State Sciences |
| Separation and Purification Technology | Sensors and Actuators B: Chemical |
| ACS Earth and Space Chemistry | Acta Materialia |
| Journal of Materials Science: Materials in Electronics | RSC Advances |
| Sustainability (MDPI) | Frontier in Chemistry |
| Transactions of the Indian Institute of Metals | Acta Materialia |
| Energies (MDPI) | Materials (MDPI) |
| Crystals (MDPI) | Applied Sciences (MDPI) |
| Coating (MDPI) | Symmetry (MDPI) |
| ChemEngineering (MDPI) | Batteries (MDPI) |