



Project Proposal for Ph.D.

Project Details	
Project Title	Molecular Dynamics and Experimental Studies on Glass-electrolytes for Application in Batteries
Project Summary (Minimum 500 and maximum 2000 characters)	Most electrolytes used in conventional metal ion batteries today are liquid-based because of adequate wetting of the electrodes, high ionic conductivity, low-interfacial resistance, and fast charging/discharging cycles. Even though liquid electrolytes are favorable to promote charge transport and electrochemical storage, the issues, such as decomposition of electrolyte, electrolyte leakage, flammability, dendritic growth pose severe challenges for safety. Recently, glass electrolytes have demonstrated highly reversible and stable operation of the metal anodes at room-temperature; however, the cell is identified to suffer immensely from the interfacial resistance. In the present proposal, bulk and interfacial properties of novel glass electrolytes will be studied using both experiments as well as molecular dynamics simulations.

Ph.D. Supervisors			
Role	Name of Faculty	Academic Unit in IITD/Institute/University	Email ID (Official)
Supervisor 1	Dr. Hemant K. Kashyap	Chemistry, IITD	hkashyap@chemistry.iitd.ac.in
Supervisor 2	Dr. Vipin Kumar	DESE, IITD	vkumar@iitd.ac.in

Project requirements (Student qualifications, experience required, etc) *The candidate will be shortlisted based on common shortlisting criteria decided by ScRC (SIRe)
M.Sc./M.Tech. in Chemistry/Physics or related areas with very good academic record

Source of fellowship/funding (CSIR/UGC/DBT/ICMR/ICAR/NEET-PG/DST-INSPIRE/IRD/FITT Project details, if any)
Candidate with his/her own fellowship /institute assistantship

Role of Faculty Members involved:	
Supervisor-1	Prof. Hemant K. Kashyap’s expertise on computational chemistry will be used to supervise the student to perform ab initio quantum chemical calculations and molecular dynamics simulations for glass electrolytes.
Supervisor-2	Prof. Vipin Kumar’s expertise on batteries will be used for experimental characterization of different glass electrolytes.