

课程大纲 COURSE SYLLABUS

1.	课程代码/名称 Course Code/Title	MSE5022 电解质基础 Fundamentals of Electrolytes
2.	课程性质 Compulsory/Elective	专业选修课
3.	课程学分/学时 Course Credit/Hours	3/48
4.	授课语言 Teaching Language	英语/English
5.	授课教师 Instructor(s)	邓永红 副教授
6.	是否面向本科生开放 Open to undergraduates or not	否
7.	先修要求 Pre-requisites	MSE301 材料化学; MSE306 材料测试分析技术
8.	教学目标 Course Objectives	
	让学生理解电解质是如何工作的, 为如何设计高性能电解质奠定基础。Let students know how electrolyte additives work in Li-ion batteries, and how to design the electrolytes with high performances	
9.	教学方法 Teaching Methods	
	本课程分课堂讲解、师生讨论、课后文献查找等环节。通过理论联系实际的训练, 让同学展示自己对重要知识点的理解和掌握程度 The course is achieved by teaching in classroom, discussing between the teacher and students, and looking up references after school. Training the students by linking theory with practice, and then let them show their understanding and mastering degree on important knowledge points	
10.	教学内容 Course Contents	
	Section 1	Introduction and Scope Electrochemistry Basics: Faraday, Nernst Volta: What is Battery? Why a Battery Is Complicated Battery basics: $E=C * V$ Components and system: What determines electrode potential? What determines capacity? What determines energy? What if “Moore’ s Law” is obeyed? The Attraction of “Lithium” and Its Challenge Why Lithium? The energy density of possible metal anodes (compare Na, Be, Mg, Al etc) The ultimate anode

	<p>The challenge:</p> <p>Reactivity and passivation</p> <p>Interphase (SEI)</p> <p>Dendrite and dead Li</p> <p>The first fiasco of Li-metal batteries (Moli, 1988)</p> <p>From “Lithium” to “Lithium Ion”</p> <p>The intercalation Bypass</p> <p>“Host-guest” chemistry (1960 concepts; 1987 Nobel prize)</p> <p>Electrochemical extension of “Host-guest” chemistry : dual-intercalation battery concept (Armand 1980)</p> <p>Whittingham (1976?):</p> <p>chalcogenides (TiS₂); stable electrochemical system: Li/TiS₂; unstable vs. moisture; low potential (2 V batteries)</p> <p>35 yrs later the battery still works</p> <p>Goodenough (1980)</p> <p>Oxides replacing chalcogenides: stable vs moisture; high potential (4 V batteries)</p> <p>LCO (1980); LMO (with Thackeray, 1985?); LiFePO₄ (with Padhi, 1997)</p> <p>Scrosati assembled the 1st LIB by concept: Transition oxides as both electrodes; 2 V</p> <p>Asahi Kasei assembled the 1st modern LIB (1986): LCO cathode; petroleum coke anode; PC electrolyte</p> <p>Sony commercialize the 1st modern LIB (1990)</p>
<p>Section 2</p>	<p>Fundamentals of Battery Electrolytes</p> <p>Electrolyte separates cathode and anode as ionic conductor:</p> <p>Conducts ionic current</p> <p>Insulates electron transport</p> <p>Facilitates mass transport</p> <p>Electrolyte requirements: ion conductor; electron insulator; medium for mass transport; electrochemically stable on both cathode and anode</p> <p>Thermodynamic stability vs kinetic stability (interphase)</p> <p>Electrolyte is ionic conductor, therefore a salt needs to be in dissociated state, so that cation and anion can move</p> <p>Ionic liquid (molten salt)</p> <p>Electrolyte solution: solvent molecules dissolve cations and anions</p> <p>Most electrolytes are liquid: good contact at interfaces</p> <p>HOMO/LUMO of electrolytes vs. redox potential of electrodes</p> <p>Lower LUMO: resistance against reduction</p> <p>Higher HOMO: resistance against oxidation</p>
<p>Section 3</p>	<p>Electrolyte Components</p> <p>Solvents: high dielectric constant (ability to dissolve salt into separate ions); low viscosity (high transport rate and high ionic mobility) , stability against reduction and oxidation at electrodes (ether: high stability vs reduction; esters: high stability vs. oxidation)</p> <p>Propylene Carbonate (PC)</p>

	<p>Ethylene Carbonate (EC)</p> <p>Linear Dialkyl Carbonates</p> <p>Other new solvents</p> <p>Salts : cations of interest to cell chemistry (eg., Li⁺ for Li-based batteries); anions with high stability with other electrolyte and cell components (especially stable against oxidation); high dissociation constant</p> <p>Lithium Perchlorate (LiClO₄)</p> <p>Lithium Hexafluoroarsenate (LiAsF₆)</p> <p>Lithium Tetrafluoroborate (LiBF₄)</p> <p>Lithium Trifluoromethanesulfonate (LiTf)</p> <p>Lithium Bis(trifluoromethanesulfonyl)imide (LiIm) and Its Derivatives</p> <p>Lithium Hexafluorophosphate (LiPF₆)</p> <p>Other new salts</p> <p>Functional Additives</p> <p>S-containing Additives</p> <p>P-containing Additives</p> <p>Si-containing Additives</p> <p>Other New Additives</p>
Section 4	<p>Electrolyte Bulk Properties</p> <p>4.1. Ion Transport</p> <p>4.2. Li⁺-Solvation</p> <p>4.3. Li⁺-Solvent Interaction in Electrolyte Solutions</p> <p>4.4. Li⁺-Solvates in Concentrated Electrolytes</p>
Section 5	<p>Interface & Interphase</p> <p>5.1 Electrolyte/Anode Interface: SEI</p> <p>Passivation on Lithium Anode</p> <p>Electrolyte/Carbonaceous Anode Interface</p> <p>Exfoliation and Irreversible Capacities on a Carbonaceous Anode</p> <p>Mechanism of SEI Formation</p> <p>5.2 Electrolyte/Cathode Interface: CEI</p> <p>Passivation Film on a Cathode</p> <p>Mechanism of SEI Formation</p> <p>5.3 Breakdown of Surface Layer</p> <p>5.4. Passivation of Current Collector</p>
Section 6	<p>6. Chemical and Thermal Stability/Safety of Electrolytes</p> <p>Long-Term Stability of Electrolytes at Elevated Temperatures</p> <p>Stability of the SEI or Surface Layer at Elevated Temperatures</p> <p>Thermal Safety of Electrolytes against Abuse</p> <p>Degradation Mechanisms</p> <p>Electrolyte Components to Suppress Degradations</p> <p>Chemical and Thermal Degradations</p> <p>Degradations with Anode</p> <p>Degradations with Cathode</p> <p>Degradations with Aluminum Substrate</p>
Section 7	<p>Characterization</p> <p>X-rayPhotoelectron Spectroscopy (XPS)</p>

	<p>GC-MS/ LC-MS spectroscopy Advanced Characterization and Imaging Ellipsometry and Sum-Frequency Generation Spectra Electron Microscopes Acoustics Neutron-Based Techniques Fluorescence Electrochemical Quartz Crystal Microbalance Scanning Probe Microscopy</p>
Section 8	<p>Novel Electrolyte Systems 8.1. Problems Facing State-of-the-Art Electrolytes 8.2.1. Anode: SEI Modification 8.2.3. Cathode: Overcharge Protection 8.3. New Electrolyte Components 8.3.1. Nonaqueous Solvents 8.3.2. Lithium Salts 8.4. Novel Electrolytes with a Wide Temperature Range 8.4.1. Low-Temperature Performance 8.4.2. High-Temperature Performance 8.5. Electrolytes of Low Flammability 8.6. Polymer and Polymer Gel Electrolytes 8.6.1. Solid Polymer Electrolyte 8.6.2. Gel Polymer Electrolyte</p>
11. 课程考核 Course Assessment	
	<p>课程考核分为三部分：期末考查：50%；其中考查20%；考勤、作业、课堂表现 30%。 Three parts for course assessments: Final Assessment: 50%; Middle Assessment: 20%; Attendance, Assignments and Classroom Performance: 30%</p>
12. 教材及其它参考资料 Textbook and Supplementary Readings	
	<p>1. Martin Winter, Brian Barnett, and Kang Xu. Before Li Ion Batteries. Chem. Rev. 2018, 118, 11433–11456 2. Kang Xu. Electrolytes and Interphases in Li-Ion Batteries and Beyond. Chem. Rev. 2014, 114, 11503 – 11618. 3. Nonaqueous Liquid Electrolytes for Lithium-Based Rechargeable Batteries. Chem. Rev. 2004, 104, 4303-4417 4. Y.H. Deng*et.al. How electrolyte additives work in Li-ion batteries, Energy Storage Materials, 2018, DOI: 10.1016/j.ensm 5. John O' M., Bockris and Amulya K.N. Reddy. 《Modern Electrochemistry 1 : Ionics》, Kluwer Academic/Plenum Publishers, 1998.6. ISBN-10: 0306455552</p>