

Sustainability in Materials Science and Engineering Education and Research

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March 28, 2016

All technologies require resources
(materials, energy) to fabricate.

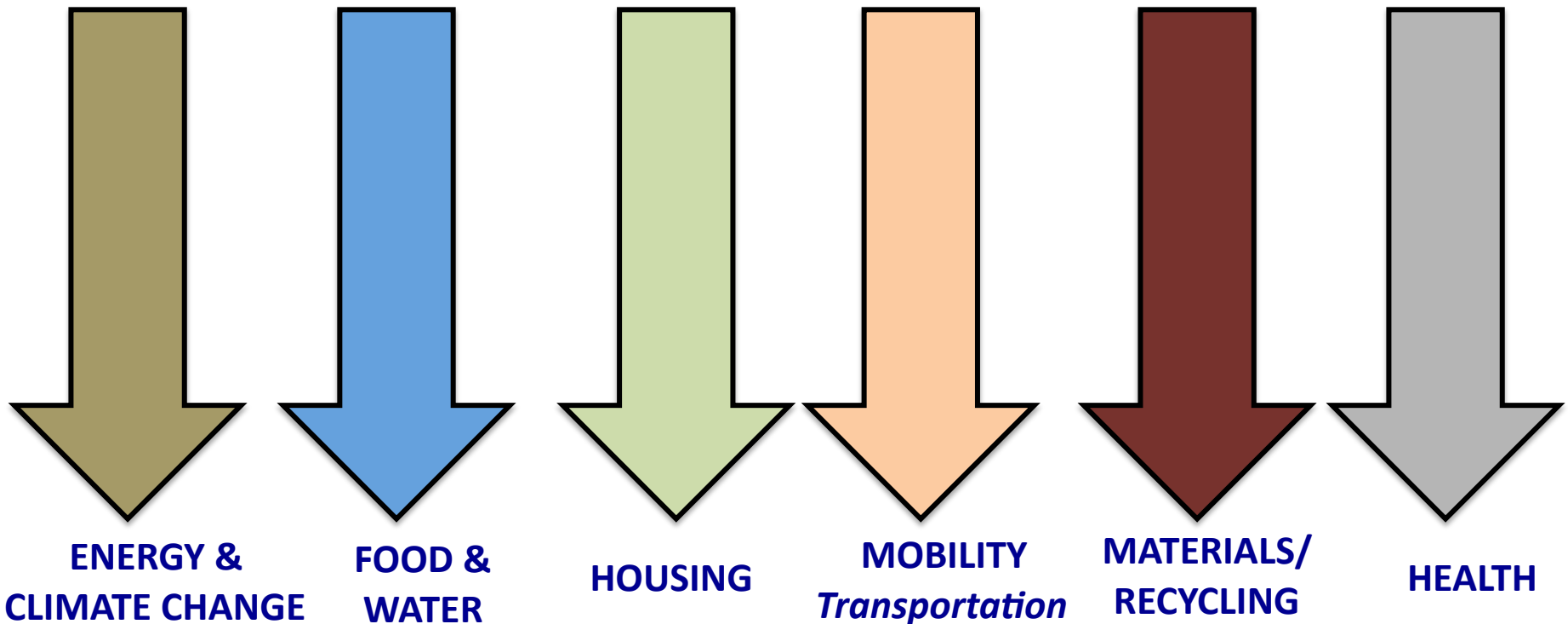
Many products require hazardous/toxic substances in the product itself and/or in the production process. Others utilize materials that are in limited supply or are difficult to recycle.

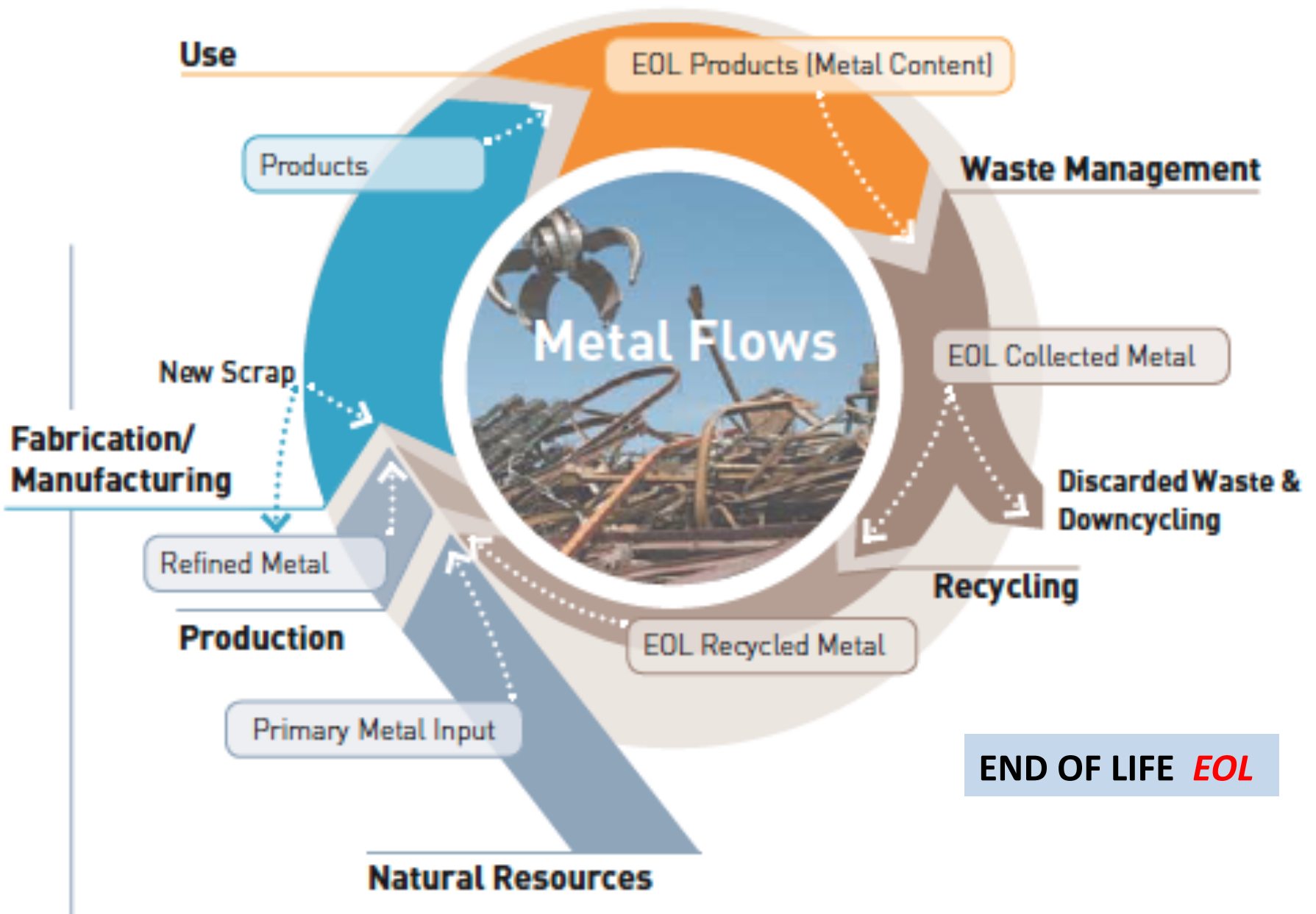
MSE students and researchers play an important role in defining product composition and processing details. They need to play a role in selecting materials and process chemicals that are not harmful to humans and the environment.

They can also become part of the community expanding sustainability assessment methodologies.

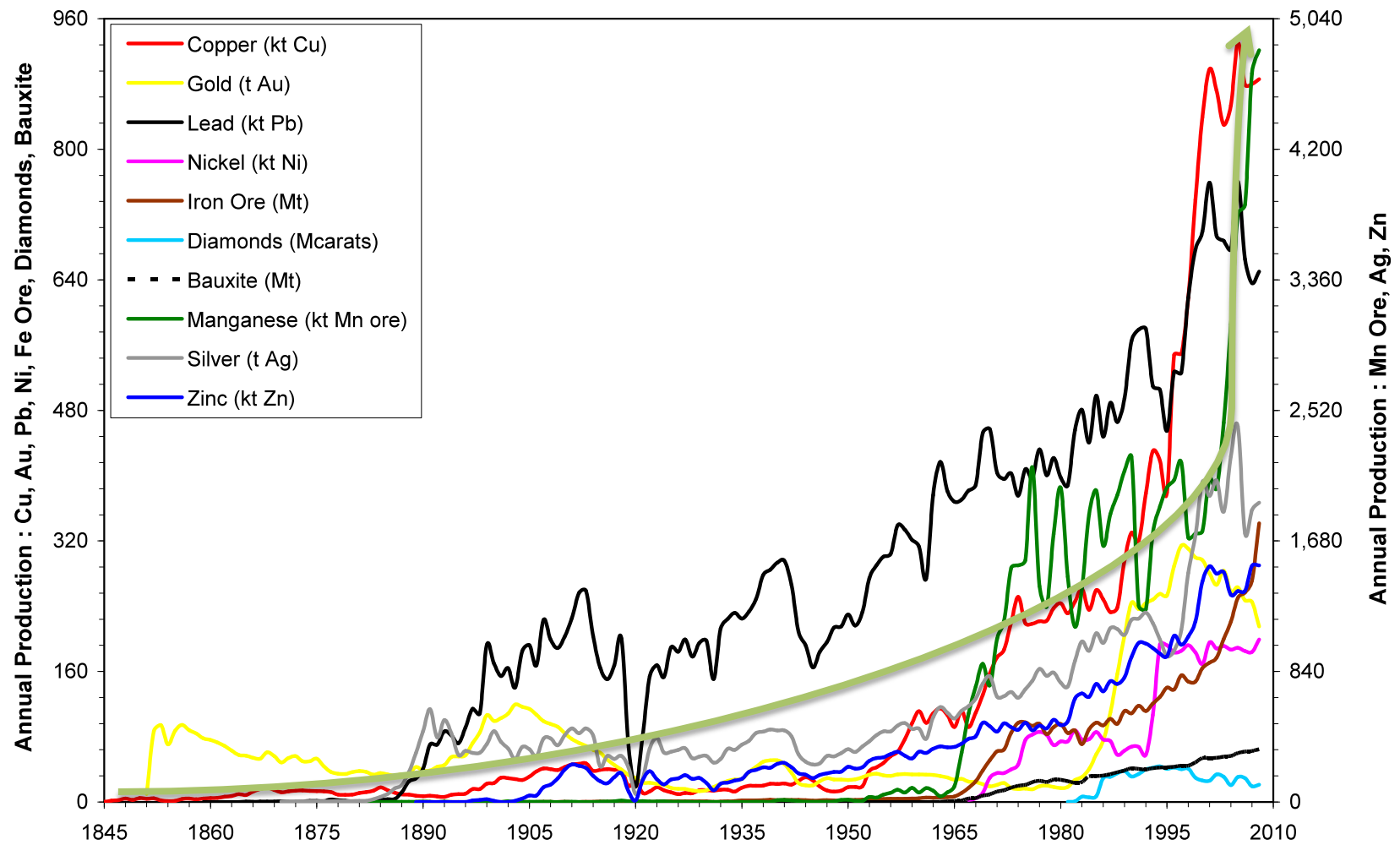
SUSTAINABLE DEVELOPMENT

SOCIETAL NEEDS - CHALLENGES

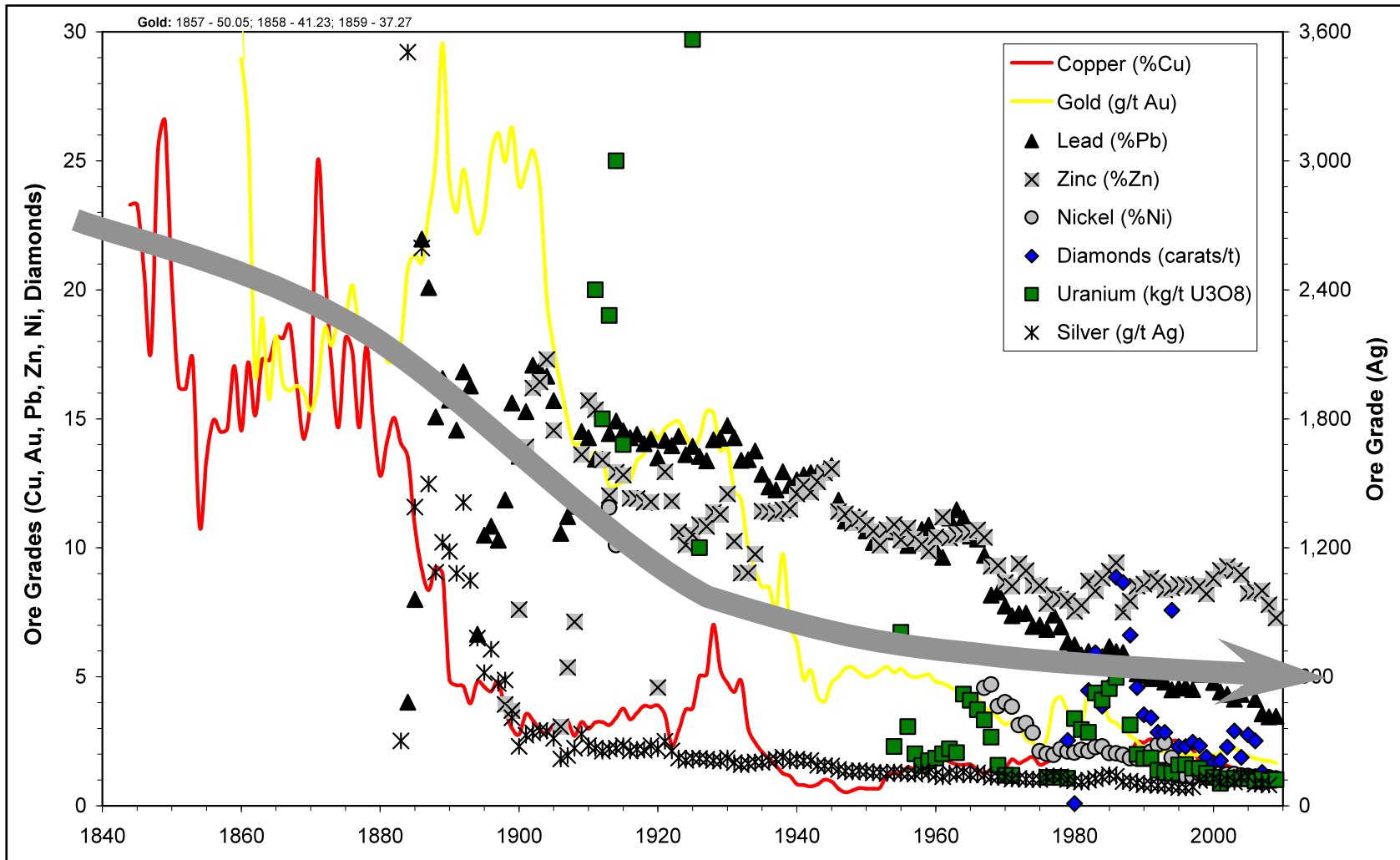




Metal Production Trends



Trends in Ore Grade



Consumer products are increasingly complex



© Umicore

- Ag, Au, Pd... (precious metals)
- Cu, Al, Ni, Sn, Zn, Fe, Bi, Sb, In... (base & special metals)
- Hg, Be, Pb, Cd, As... (metals of concern!)
- halogens (Br, F, Cl...)
- plastics & other organics
- Glass, ceramics

These devices represent a considerable metal stock in society

Cell phones*:

1300 Million units x 250 mg Ag \approx 325 t Ag
 x 24 mg Au \approx 31 t Au
 x 9 mg Pd \approx 12 t Pd
 x 9 g Cu \approx 12,000 t Cu
 x 3.8 g Co¹ \approx 4900 t Co

PC & laptops*:

300 Million units x 1000 mg Ag \approx 300 t Ag
 x 220 mg Au \approx 66 t Au
 x 80 mg Pd \approx 24 t Pd
 x \approx 500 g Cu \approx 150,000 t Cu
 \approx 140 M batteries² x 65 g Co \approx 9100 t Co

* based on 2008 sales, Gartner 2.3.2009

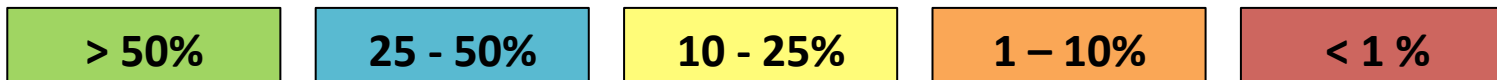
¹ 20 g Li-ion battery

² Li-ion batteries is used in >90% of laptops

Credit: C. Meskers - Umicore

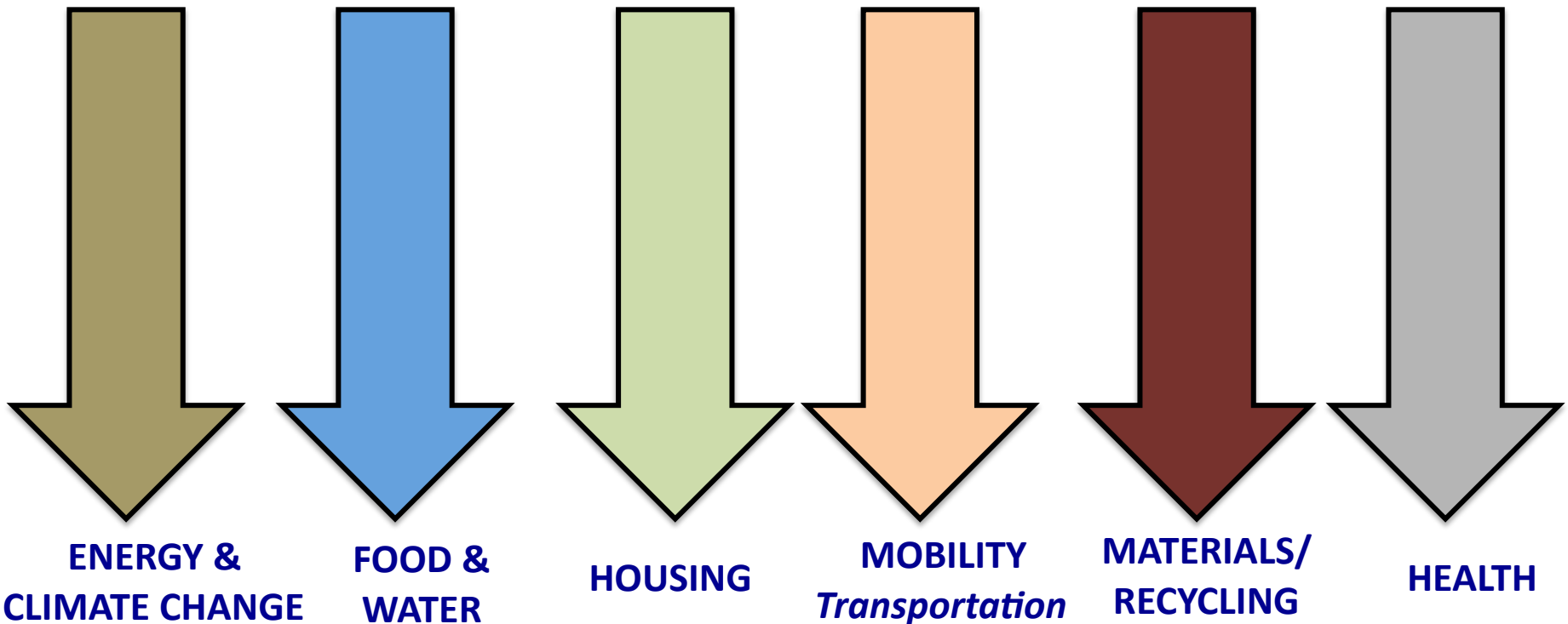
End-of-life Recycling Rates

H																	He																														
Li	Be											B	C	N	O	F	Ne																														
Na	Mg											Al	Si	P	S	Cl	Ar																														
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																														
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																														
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																														
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Uuq	Uup	Uuh	Uus	Uuo																														
<table border="1"> <tr> <td>La</td><td>Ce</td><td>Pr</td><td>Nd</td><td>Pm</td><td>Sm</td><td>Eu</td><td>Gd</td><td>Tb</td><td>Dy</td><td>Ho</td><td>Er</td><td>Tm</td><td>Yb</td><td>Lu</td> </tr> <tr> <td>Ac</td><td>Th</td><td>Pa</td><td>U</td><td>Np</td><td>Pu</td><td>Am</td><td>Cm</td><td>Bk</td><td>Cf</td><td>Es</td><td>Fm</td><td>Md</td><td>No</td><td>Lr</td> </tr> </table>																		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																																	
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SUSTAINABLE DEVELOPMENT

SOCIETAL NEEDS - CHALLENGES



Toxicity Characteristic Leaching Procedure (TCLP) Regulatory Levels

METALS	TCLP Regulatory Level, mg/L	EPA Hazardous Waste Number	Recommended Test Method
Arsenic	5.0	D004	7061
Barium	100.0	D005	7080
Cadmium	1.0	D006	7130
Chromium	5.0	D007	7190
Lead	5.0	D008	7420
Mercury	0.2	D009	7471
Selenium	1.0	D010	7741
Silver	5.0	D011	7760

High values are preferred.

Reference: 40 CFR 261, Appendix II, 1993 ed., as amended by 58 FR 46040, August 31, 1993.

Leachability Test: LED Diodes

- TTLc results for State of California hazardous waste classification (units mg/kg)
 "N/A" : Not Applicable, "-" : Not Detected; Low Values are Preferred; High Thresholds are Less Hazardous

Substance	TTLc Threshold	LED (color/intensity)								
		Red /Low	Red /High	Yellow /Low	Yellow /High	Green /Low	Green /High	Blue /Low	Blue /High	White
Aluminum	N/A	97.0	158.0	104.0	156.0	79.6	156.0	153.0	73.4	84.5
Antimony	500	15.4	2.0	2.8	1.9	3.6	2.5	1.3	1.5	25.9
Arsenic	500	11.8	111.0	8.0	84.6	7.8	15.2	5.7	5.4	-
Barium	10000	-	-	-	-	-	-	-	-	-
Cerium	N/A	-	-	-	-	-	-	-	-	-
Chromium	500(VI);2500(III)	138.0	28.6	32.7	27.9	84.1	49.3	50.9	30.3	65.9
Copper	2500	87.0	3818.0	956.0	2948.0	1697.0	3702.0	3892.0	2153.0	31.8
Gadolinium	N/A	-	-	-	-	-	-	-	-	-
Gallium	N/A	135.6	95.0	63.8	79.1	75.6	3.1	2.1	1.5	3.8
Gold	N/A	39.8	45.8	30.5	30.1	40.2	176.3	32.5	118.6	115.9
Indium	N/A	3.4	1.7	-	-	2.5	-	-	-	-
Iron	N/A	285558.2	363890.8	300905.6	398630.4	310720.6	395652.2	339234.5	256499.3	311303.6
Lead	1000	8103.0	8.9	7.7	-	5.0	-	-	-	-
Mercury	20	-	-	-	-	-	-	-	-	-
Nickel	2000	4797.0	2054.0	1541.0	2192.0	2442.0	2930.0	1564.0	1741.0	4083.0
Phosphorus	N/A	114.2	-	58.4	-	78.5	91.8	79.1	84.3	110.8
Silver	500	430.0	409.0	248.0	336.0	270.0	306.0	418.0	721.0	520.0
Tungsten	N/A	-	-	-	-	-	-	-	-	-
Yttrium	N/A	-	-	-	-	-	-	-	-	-
Zinc	5000	48.2	66.2	36.5	63.6	41.8	62.5	42.6	36.7	49.2

Table I. Environmental releases (2009) and human health toxicity indices for selected chemicals.^{a,b}

	Total TRI ¹⁰ releases in 2009 (kg)	Human exposure limits ^{c,11,12}			IARC classification ^{d,13}	NTP classification
		PEL (mg/m ³)	TLV (mg/m ³)	REL (mg/m ³)		
Metals						
Aluminum	11,400,000	5	1	10	–	–
Antimony	444,000	0.5	0.5	0.5	–	–
Arsenic	339,000	0.01	0.01	–	Group 1	Known carcinogen
Barium	2,310,000	0.5	0.5	0.5	–	–
Beryllium	4730	0.002	0.00005	–	Group 1	Known carcinogen
Cadmium	183,000	0.005	0.002	0.1	Group 1	Known carcinogen
Chromium	3,610,000	0.5	0.5	0.5	Group 3	–
Cobalt	135,000	0.1	0.02	0.05	Group 2B	–
Copper	4,440,000	0.1	0.2	0.1	–	–
Lead	6,480,000	0.05	0.05	0.05	Group 2B	Anticipated carcinogen
Manganese	6,420,000	–	0.2	1	–	–
Mercury	56,000	–	0.025	0.05	Group 3	–
Nickel	2,330,000	1	1.5	0.015	Group 2B	Anticipated carcinogen
Selenium	65,000	0.2	0.2	0.2	Group 3	–
Silver	62,000	0.01	0.1	0.01	–	–
Thallium	171	0.1	0.1	0.1	–	–
Vanadium	945,000	–	–	–	–	–
Zinc	5,400,000	–	–	–	–	–

^aAcronyms: IARC, International Agency for Research on Cancer; NTP, National Toxicology Program; PEL, permissible exposure limit; REL, reference exposure level; TLV, threshold limit value; TRI, Toxics Release Inventory.

^bCells highlighted in rose contain quantitative or qualitative information sufficient to trigger caution in using the corresponding chemicals in manufacturing.

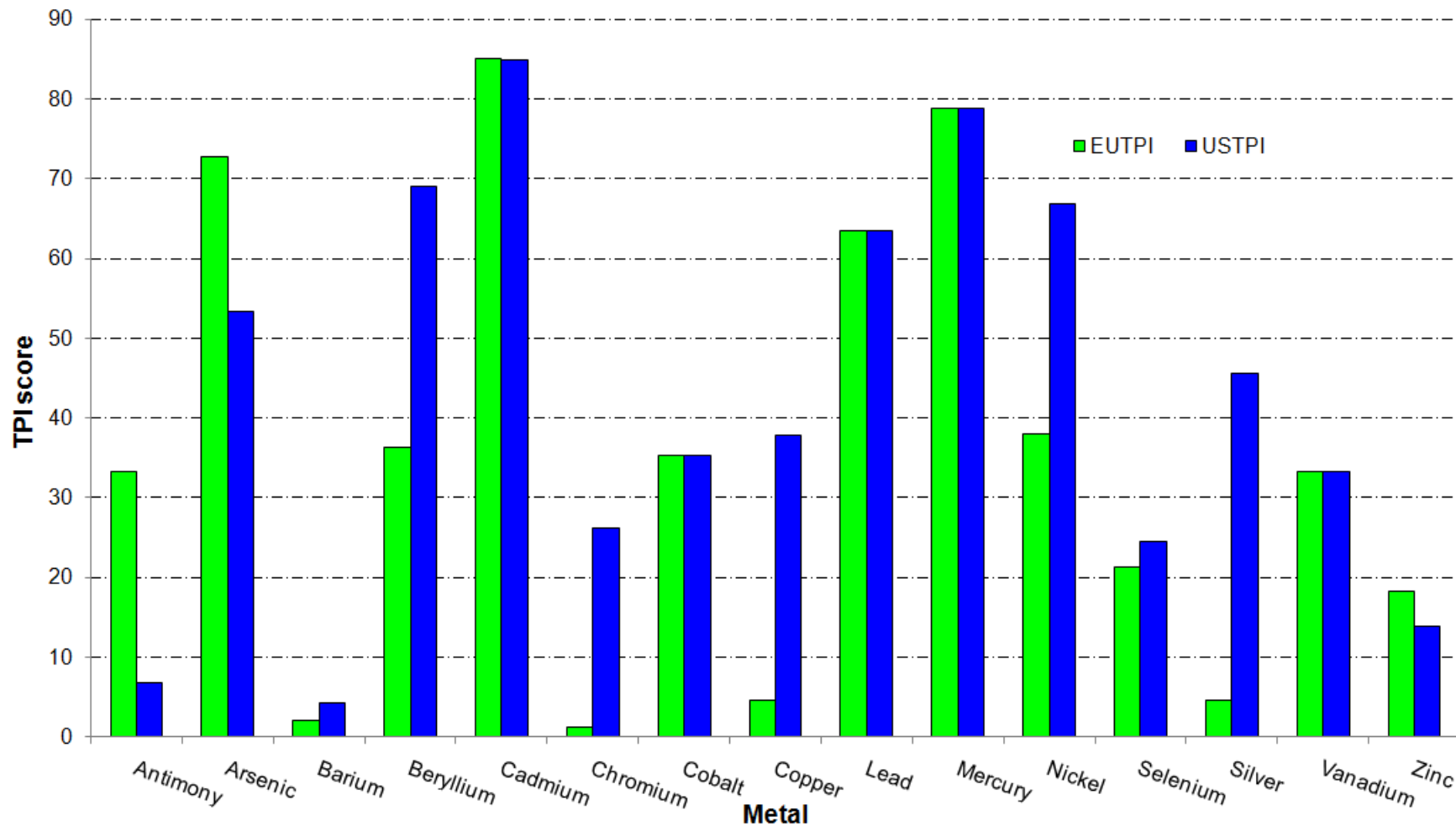
^cHigh values are preferred for PEL, TLV, and REL.

^dThe specific IARC group classifications are as follows: Group 1, carcinogenic to humans; Group 2A, probably carcinogenic to humans; Group 2B, possibly carcinogenic to humans; Group 3, not classifiable as to carcinogenicity to humans; and Group 4, probably not carcinogenic to humans.

Toxic Potential Indicator (TPI) Scores for Metals

Derived from: human health, environmental health and physical hazards

Low scores are preferred; possible range is 0-100



GreenScreen® Provisional Benchmark Scores

“Provisional”: not reviewed by toxicologist; derived from GHS Japan data only

1 H 1.008																	2 He 4.0026
3 Li 6.94	4 Be 9.0122											5 B 10.81	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.085	15 P 30.974	16 S 32.06	17 Cl 35.45	18 Ar 39.948
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.63	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.798
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.96	43 Tc [97.91]	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	* 71 Lu 174.97	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po [208.98]	85 At [209.99]	86 Rn [222.02]
87 Fr [223.02]	88 Ra [226.03]	** 103 Lr [262.11]	104 Rf [265.12]	105 Db [268.13]	106 Sg [271.13]	107 Bh [270]	108 Hs [277.15]	109 Mt [276.15]	110 Ds [281.16]	111 Rg [280.16]	112 Cn [285.17]	113 Uut [284.18]	114 Fl [289.19]	115 Uup [288.19]	116 Lv [293]	117 Uus [294]	118 Uuo [294]
*Lanthanoids		* 57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm [144.91]	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05		
**Actinoids		** 89 Ac [227.03]	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np [237.05]	94 Pu [244.06]	95 Am [243.06]	96 Cm [247.07]	97 Bk [247.07]	98 Cf [251.08]	99 Es [252.08]	100 Fm [257.10]	101 Md [258.10]	102 No [259.10]		

Benchmark 3: Use but Still Opportunity for Improvement

Benchmark 2: Use but Search for Safer Substitutes

Benchmark 4: Safer Chemical

Benchmark 1: Chemical of High Concern

Benchmark U: Unspecified due to Data Gaps

(Derived from data in: K. Wehage, P. Chenhansa, J.M. Schoenung, “An Open Framework for Automated Chemical Hazard Assessment based on GreenScreen for Safer Chemicals,” *Integrated Environmental Assessment and Management*, in press 2016; GreenScreen for Safer Chemicals® methodology developed by Clean Production Action)

GreenScreen for Safer Chemicals[®]:

Hazard Traits

Priority Human Health Effects (PE)	Human Health Effects (HH)	Ecotoxicity (Eco)	Environmental Fate (EF)	Physical Hazards (Phy)
Carcinogenicity (C)	Acute Toxicity (AT)	Acute Aquatic Toxicity (AA)	Persistence (P)	Explosivity (E)
Mutagenicity (M)	Irritation and Corrosion (IC)	Chronic Aquatic Toxicity (CA)	Bioaccumulation (B)	Flammability (F)
Reproductive (R)	Skin/Eye Sensitization (S)			
Developmental (D)	Immune System effects (IS)			
Endocrine Disruption (ED)	Systemic Organ Toxicity (SOT)			
Neurological (N)				

Utilizes 17 hazard traits from UN's GHS for hazard assessment

Thin Film Solar Cells

CIGS Deposition: Assessment Results

Hazard: Low \longrightarrow High Low \longrightarrow High

CIGS Deposition Process		GS-Based Benchmark frequency				TPI score frequency			
Type of Processing	Specific Deposition Method	4	3	2	1	low	mid	high	very high
Industrial Process	Coevaporation	0	1	4	0	1	1	2	1
Ink Printing	Spray Pyrolysis of CuInS_2	0	0	2	1	0	0	3	0
Electrodeposition	Kapmann Method	1	1	4	2	2	0	5	1
Industrial Process	Sulfurization/ Selenization	1	1	4	1	1	1	3	1
Chemical Vapor Deposition	AP-MOCVD	0	0	6	1	3	0	2	1
Electrodeposition	Kapmann Method with Ammonia	1	1	4	3	2	1	5	1

D.A. Eisenberg, MYu, C.W. Lam, O.A. Ogunseitan, J.M. Schoenung, "Comparative Alternative Materials Assessment to Minimize Toxicity Hazards in the Life Cycle of Thin Film Photovoltaics," *Journal of Hazardous Materials* 260 (2013) 534-542.

Toxicity Potential Summary: **Bulbs** 🎵

- Comparison of the incandescent, CFL, and LED bulbs taking into account design lifetimes (1000, 10,000, 50,000 hr, respectively).

Low values are preferred.

Environmental Impact Assessment Category and Method		Incandescent Bulb	CFL Bulb	LED Bulb	
Resource Depletion Potential	CML 2001	1	3	3	
	EPS 2000	1	5	2	
Hazard-based Toxicity Potential	TLV-TWA	1	4	3	
	PEL-TWA	1	13	3	
	REL-TWA	1	8	2	
	TPI	1	16	2	
Life Cycle Impact (USEtox™)-based Toxicity Potential	Human-Toxicity Potential	Urban Air	1	22	2
		Rural Air	1	22	2
		Freshwater	1	25	2
		Sea Water	1	22	2
		Natural Soil	1	26	2
		Agricultural Soil	1	22	2
	Eco-toxicity Potential	Urban Air	1	22	3
		Rural Air	1	22	3
		Freshwater	1	22	3
		Sea Water	1	23	2
		Natural Soil	1	22	3
		Agricultural Soil	1	22	3

S-R. Lim, D. Kang, O.A. Ogunseitan, J.M. Schoenung, "Potential Environmental Impacts from the Metals in Incandescent, Compact Fluorescent Lamp (CFL) and Light-Emitting Diode (LED) Bulbs," *Environmental Science & Technology*, 47: 1040-1047 (2013).

UNIVERSITY OF CALIFORNIA, IRVINE
Department of Chemical Engineering & Materials Science

CBEMS 195 & 249: Green Engineering: Theory and Practice

COURSE OUTLINE

Fall 2015

Objectives: Study of the methods and impacts of selecting alternative technologies, processes, materials, chemicals, and/or products so as to reduce the pollution, waste and the use of toxic substances, thereby creating “green,” environmentally responsible, and sustainable solutions. Topics include environmental regulations, recycling, life-cycle assessment, economic analysis, design for the environment, green chemistry and toxicology.

<u>Grading:</u>	Attendance and Participation	20%
	Current Event Journal	20%
	Assignments	20%
	Quizzes	20%
	Project	20%

UNIVERSITY OF CALIFORNIA, IRVINE
Department of Chemical Engineering & Materials Science

CBEMS 195 & 249: Green Engineering: Theory and Practice

TENTATIVE LIST OF TOPICS/SPEAKERS

Fall 2015

Topics:

Introduction to Green Engineering/Green Chemistry/Pollution Prevention
Human Health Risk Assessment
Occupational Exposure
Hazard Traits: EPA DfE, GHS, OEHHA
Screening Tools and Checklists
Life Cycle Assessment (LCA)
Life Cycle Impact Assessment (LCIA)
Data Sources and Decision-Making Tools
Recycling, Recovery, Reuse
Environmental Law; State, Federal and International Initiatives

Possible Case Studies:

Electronics
Buildings
Foods/Beverages
Soaps/Shampoos/Cleaning Products/Cosmetics
Critical Materials

All technologies require resources
(materials, energy) to fabricate.

Many products require hazardous/toxic substances in the product itself and/or in the production process. Others utilize materials that are in limited supply or are difficult to recycle.

MSE students and researchers play an important role in defining product composition and processing details. They need to play a role in selecting materials and process chemicals that are not harmful to humans and the environment.

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