Sustainable Mobility, Future Fuels and the Periodic Table

Presentation Materials

What properties do we desire in a fuel?

- **Prefer not to carry more than one reactant on vehicle; take second reactant from the atmosphere.**
  - Air is 78% N_2, 21% O_2, 1% Ar. N_2 is poor reactant (N≡N bond too strong), Ar is unreactive, leaves O_2.

- **Fuel should have highly exothermic reaction with O_2**
  - … but not at ambient temperature (kinetics and thermochemistry).

- **Fuel should have high gravimetric and volumetric energy density.**

- **Fuel and exhaust should be easy to handle (i.e., liquid or gas [not solid] over "typical" temperature operation range of -20 to +40 ^oC).**

- **Exhaust should be non-toxic and unreactive with air or water**.

- **Fuel should be abundant in nature or easy to make.**
  - We need millions of tons every day.

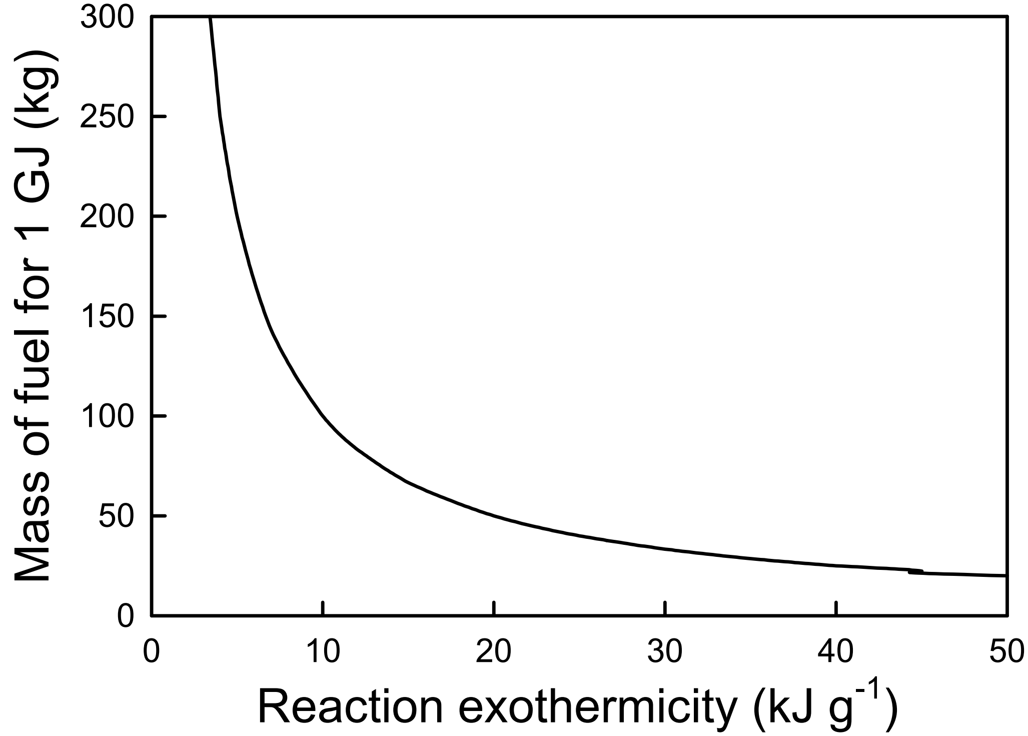
- **Fuel itself should be environmentally benign and renewable**

Periodic Table

1 **H**																	2 **He**
3 **Li**	4 **Be**											5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
11 **Na**	12 **Mg**											13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
19 **K**	20 **Ca**	21 **Sc**	22 **Ti**	23 **V**	24 **Cr**	25 **Mn**	26 **Fe**	27 **Co**	28 **Ni**	29 **Cu**	30 **Zn**	31 **Ga**	32 **Ge**	33 **As**	34 **Se**	35 **Br**	36 **Kr**
37 **Rb**	38 **Sr**	39 **Y**	40 **Zr**	41 **Nb**	42 **Mo**	43 **Tc**	44 **Ru**	45 **Rh**	46 **Pd**	47 **Ag**	48 **Cd**	49 **In**	50 **Sn**	51 **Sb**	52 **Te**	53 **I**	54 **Xe**
55 **Cs**	56 **Ba**	*	72 **Hf**	73 **Ta**	74 **W**	75 **Re**	76 **Os**	77 **Ir**	78 **Pt**	79 **Au**	80 **Hg**	81 **Tl**	82 **Pb**	83 **Bi**	84 **Po**	85 **At**	86 **Rn**
87 **Fr**	88 **Ra**	**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110 **Ds**	111 **Rg**	112 **Cn**	113 **Uut**	114 **Fl**	115 **Uup**	116 **Lv**	117 **Uus**	118 **Uuo**

*	57 **La**	58 **Ce**	59 **Pr**	60 **Nd**	61 **Pm**	62 **Sm**	63 **Eu**	64 **Gd**	65 **Tb**	66 **Dy**	67 **Ho**	68 **Er**	69 **Tm**	70 **Yb**	71 **Lu**
**	89 **Ac**	90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**

On-board fuel requirements

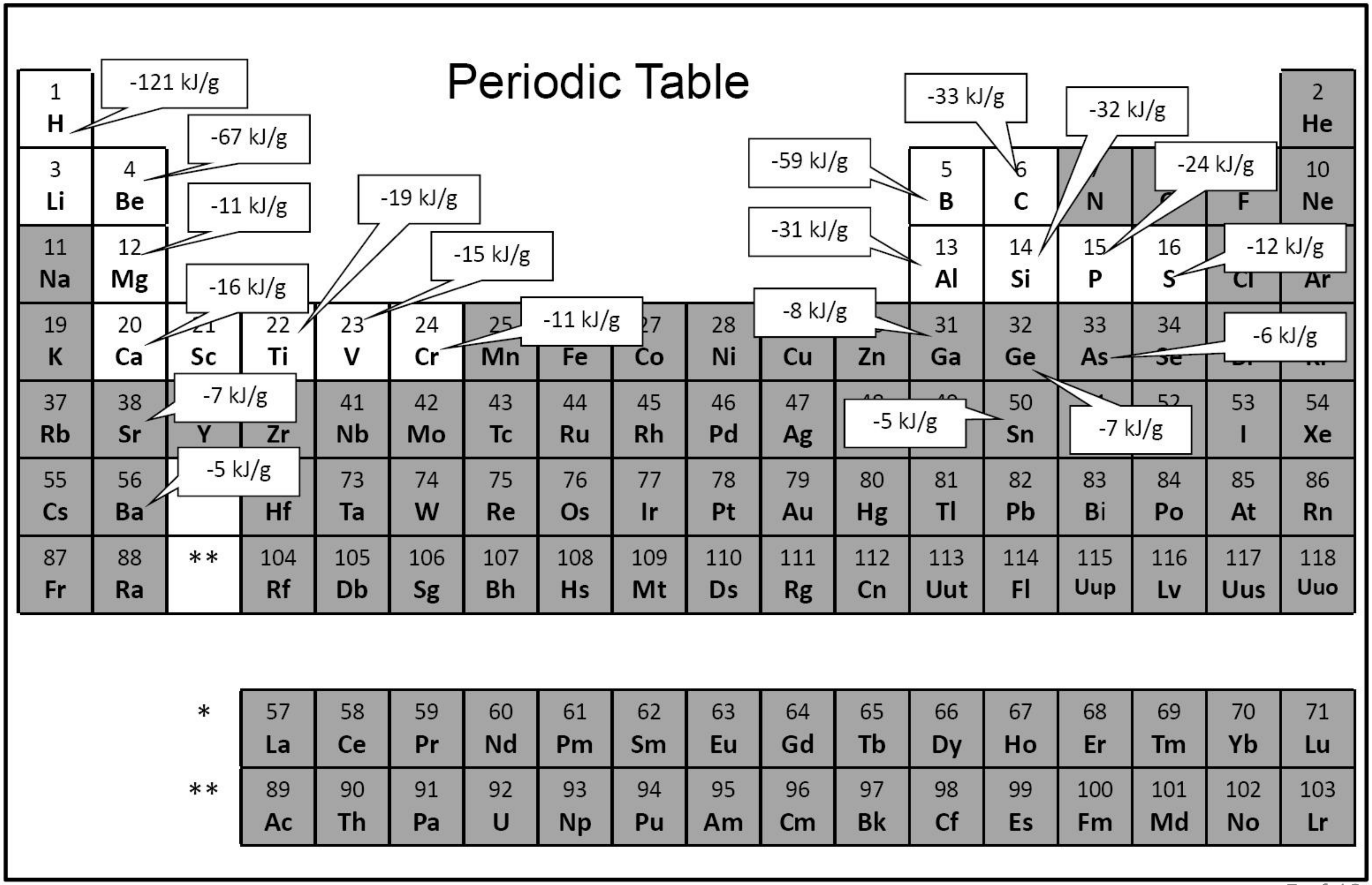


* 10-20 gallons of gasoline weighs approximately 30-60 kg, and releases approximately 45 kJ/g.

Need to carry about 1-2 GJ (equivalent to approx.10-20 gallons of gasoline*) to match functionality of current vehicles. Impractical to carry > 100 kg fuel. Hence, fuel needs to release > 10 kJ/g (preferably >> 10 kJ/g)

Highly endothermic compounds tend to be unstable. Equate maximum exothermicity of oxidation of compounds with exothermicity of oxidation of their constituent elements

Elements with enthalpy of oxidation greater than 10 kJ per gram



Elements with non-solid oxides

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37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo

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Elements left after eliminating those with: .
(i) solid oxides, (ii) low heat release on oxidation, and (iii) toxic oxides.

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Oxygenated fuels

Oxygen is not desirable from a gravimetric and volumetric energy density standpoint, but its presence can be very useful in other respects. Oxygenated fuels tend to have lower emissions of carbon monoxide, soot, and unburned hydrocarbons. Also, the hydrogen bonding in liquid oxygenated fuels results in enhanced evaporative cooling when liquid fuel is sprayed into the engine which decreases the likelihood of autoignition and hence increases fuel octane value.

Biomass feedstocks contain oxygen (glucose = $C_6H_{12}O_6$, cellulose = glucose polymer = $(C_6H_{10}O_5)_n$). Transformation processes converting biomass into fuels generally target a reduction in oxygen content, but perhaps it is not necessary, or desirable, to remove all the oxygen.

Include oxygen because oxygenates have combustion chemistry advantages in spark-ignited engines and are conveniently derived from biomass.

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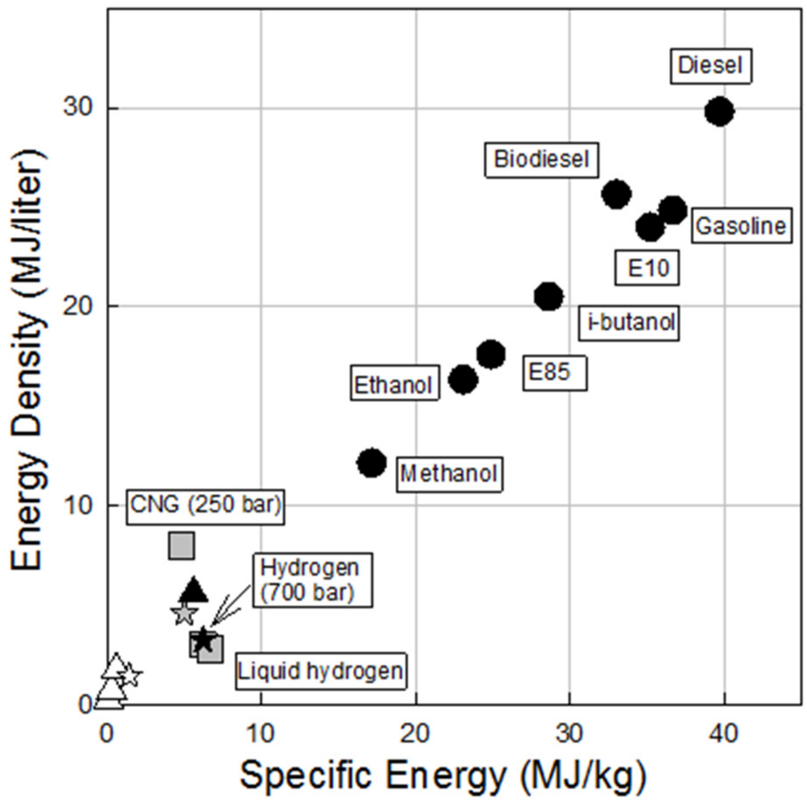
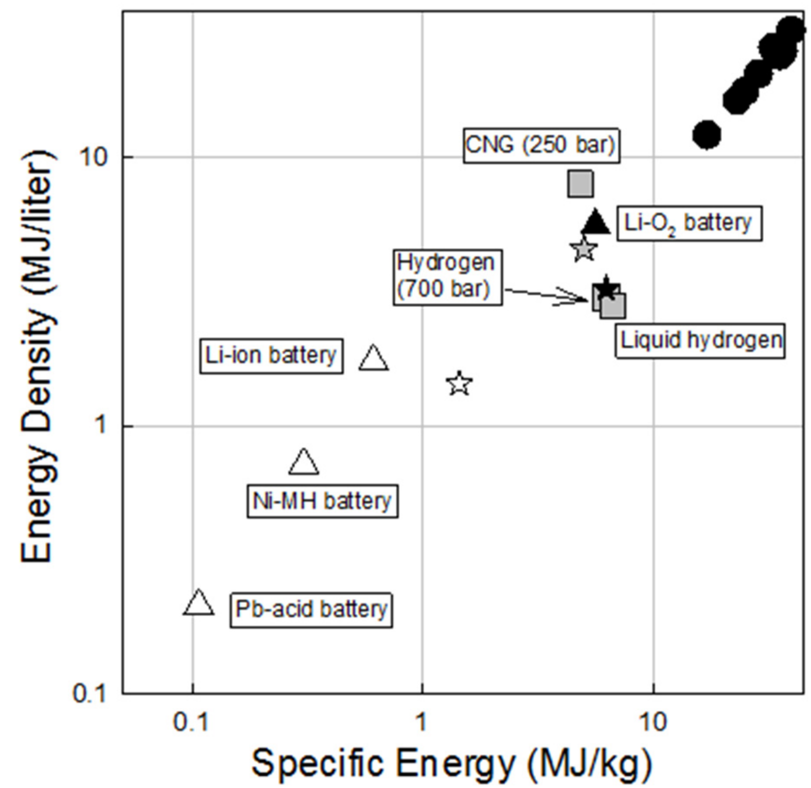
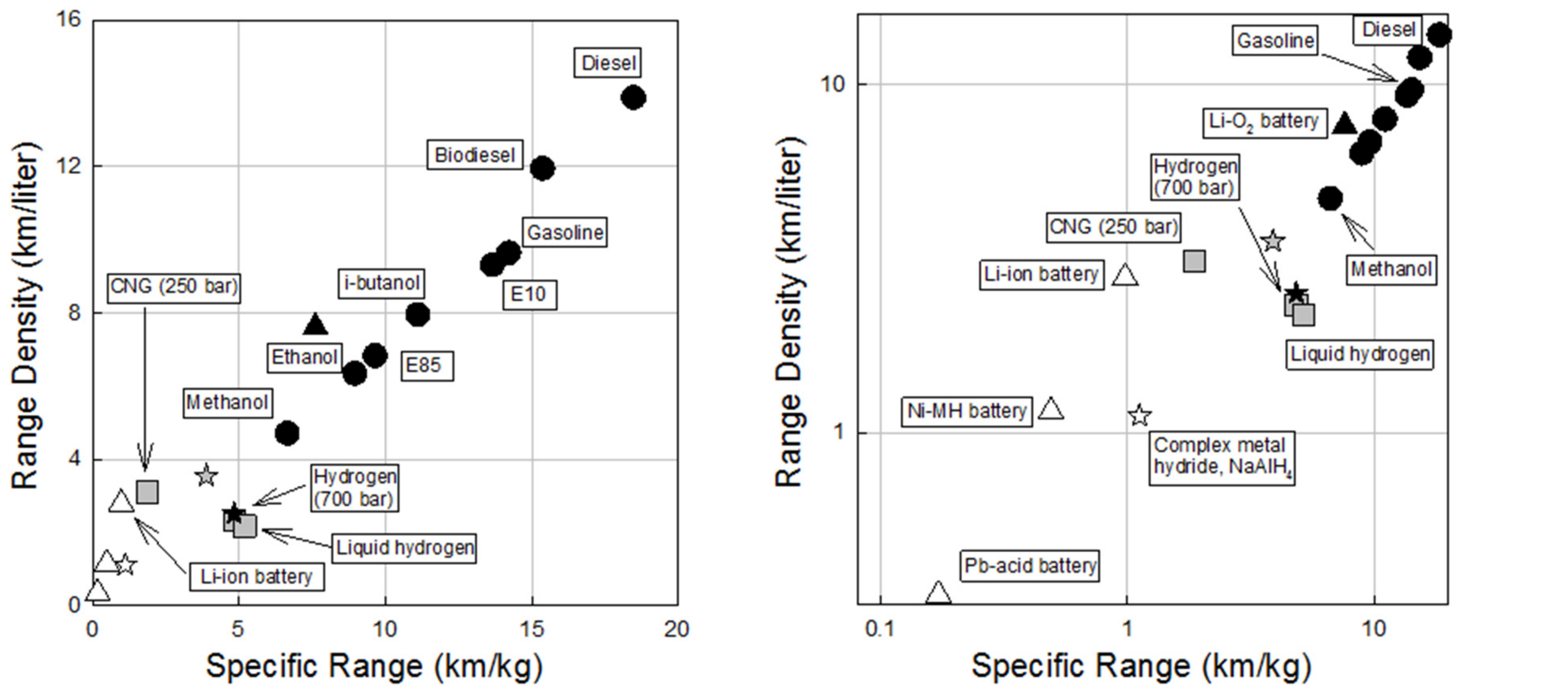
Energy density and specific energy for selected fuels





Energy density (MJ/liter) and specific energy (MJ/kg) are important parameters for a fuel. **Liquids are easy to package.**

Volumetric and gravimetric range densities for selected fuels



Alternative fuels will be compounds of H, C, possibly O and preferably liquids. With developments in battery technologies, electricity is becoming an attractive fuel.

Conclusions

- Chemical trends in the periodic table and simple physics explain the current dominance of liquid hydrocarbons as transportation fuels.
- Sustainable mobility will be powered by low-CO_2 hydrogen, low-CO_2 hydrocarbons, low-CO_2 oxygenates, low-CO_2 electricity, or a combination of the above.