GREEN SOLVENTS SELECTED BY HSP AND OTHER APPROACHES FOR PSC PRODUCTION

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ABSTRACT

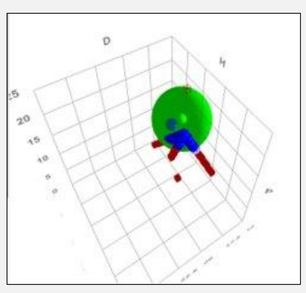
New environmentally friendly materials and processes are being globally demanded to develop **large area, low cost and flexible** solar cells such as **Perovskite Solar Cells** (PSC) with less ecological impact and manufactured by industrially up-scalable processes. **Hazardous solvents** as DMF have been classically used in the deposition of perovskite solutions for manufacturing PSCs on a laboratory scale. **Hansen Solubility Parameters (HSP**) approach has been used to identify **non-toxic solvents** that solubilize PbI_2 in order to prepare PSC with less hazardous substances in their future manufacturing process. In addition, Guttman Donor Number, Mayer Bond Order and Structural Similarity approach have been also considered to find the best candidates. A comprehensive study of non-toxic non-hazardous green solvents of perovskite precursors have been carried out in the APOLO project.

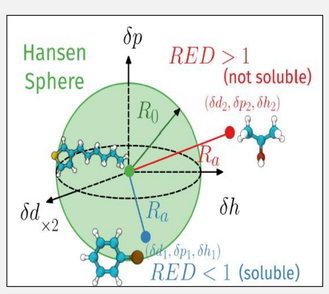
RESULTS

A) HSP: Determination of HSP by binary solvent method (PbI_2 at 400 mg/ml) to replace DMF

Common Solvents: 1247
Solvents in the junction: 19
Non-halogenated:19
MP ≤ 30°C; BP ≤200°C: 7
Toxicity: 2
Purity (≥ 98%); availability; Price: 2

1 solvents is selected: **SH1**





DMF:DMSO as reference solvents mixture
Objective: replace DMF and lower % DMSO

B) Alternative Models to HSP:

1) Mayer Bond order

Solubility governed by formation of complexes
Complexation controlled by dative bonding
Mayer Bond order: quantifying the electronic state of solvent's most electronegative atom

MP ≤ 25ºC; BP ≤200ºC: 8
Toxicity: 2

2 solvents are selected: **SM2, SM3**

2) Lewis basicity

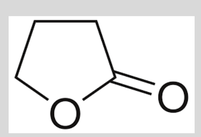
Guttman Donor Number as an indicator of Lewis basicity
Solvents having D_N> 18KCal/mol are effective solubilizing PSK precursors

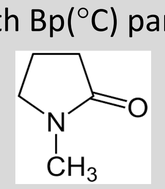
DN>18 Kcal: 23
Non-halogenated: 21
MP ≤ 25ºC; BP ≤200ºC: 17
Toxicity: 5

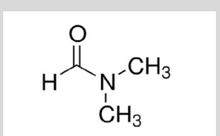
3 solvents are selected: **SL4, SL5, SL6**

3) structure similarity

Solvents having a similar structure to **GBL, DMF, NMP**
Non toxic properties
Less restrictive with Bp(°C) parameters





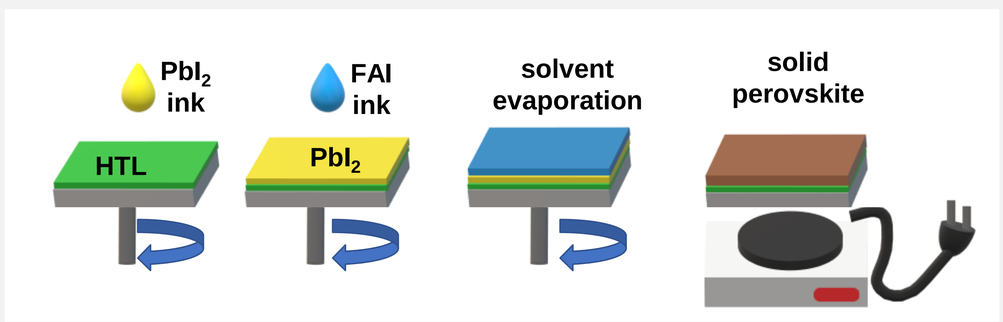


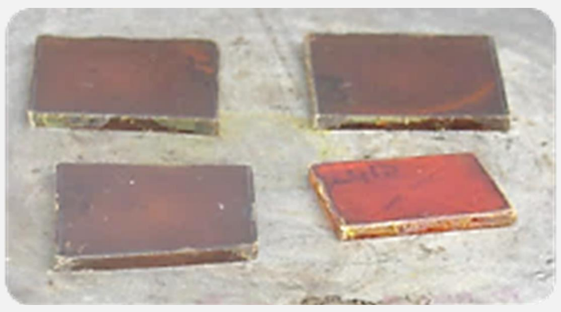
Similar to GBL (~GBL): **SS7, SS8(SL6), SS9**

Similar to NMP (~NMP): **SS10, SS11**

Similar to DMF (~DMF): **SS12, SS13, SS14**

PbI_2 400mg/ml	BINARY BLENDS												
	SH1	SM2	SM3	SL4	SL5	SL6=SS8	SS7	SS9	SS10	SS11	SS12	SS13	SS14
Model	HS	Mayer Bond	Mayer Bond	D_N	D_N	D_N	~GBL	~GBL	~NMP	~NMP	~DMF	~DMF	~DMF
Pure solvent	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
20% DMSO	✗	✗	✓	✗	+	✓	+	✗	✓	✓	✗	✗	✗
10% DMSO	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✗	✗





CONCLUSIONS

- ✓ **HSP, MBO, GDN** and **structural similarity** were used as a tools to evaluate the **PbI_2 solubility** in potential **green solvent** candidates.
- ✓ After evaluating the solubility of candidates and their blends with DMSO, trials with 4 of them presented promising results at higher concentrations 400 mg/ml with only 20-10% DMSO.
- ✓ PbI_2 thin films based on the most promising green solvents were also preliminary evaluated. An interdiffusion method carried out in a **2 steps processing** was followed for the fabrication of double cation Cs-FA PVK films.

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