Poster Presentations

[MS37-P08] PCA and DOE analysis of intercalation yield into hydrotalcites by liquid assisted grinding Marco Milanesio,[a] Eleonora Conterosito,[a] Valentina Toson,[a] Valentina Gianotti,[a] Luca Palin,[a] Gianluca Croce,[a] Claudia

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Barolo,Davide Saccone,Nadia Barbero, Giulia Magnano,Giorgio Volpi, Iacopo Benesperi,; Università del Piemonte Orientale, Italy,

[b] *Università di Torino, Italy,* E-mail: marco.milanesio@unipmn.it.

Photoactive materials can be exploited in different ways in photovoltaic fields. They can be used as direct solar light harvesters in dye sensitized solar cell or indirectly to obtain the so called "light management", i.e. the process of selecting the electro-magnetic band width more suitable for conversion to electricity. For silicon-based solar cell the desired materials adsorbs light in the high energy region of solar spectrum (below 420 nm) and emits in the middle (550 nm) where silicon is more efficient in charge separation and electricity production. This process is called "downshifting". In the present work facile production of low cost, stable and efficient downshifting materials, based on organic molecules inserted into hydrotalcite is presented. The recently developed liquid assisted grinding (LAG) method of fast and facile preparation of organic-intercalated LDH nanocomposites (Conterosito et al., Cryst Growth & Des., 2013, *13* (3), 1162) was employed to produce new photoactive hybrid materials and to screen the organic compounds that most likely undergo easy intercalation. The intercalation of dyes for DSSC cells and of materials for light downshifting to improve photovoltaic module yields was explored. Two novel molecules, (2E)-2-cyano-3-[4(dimethylamino)phenyl]prop-2-enoic acid (Dye B) and 5-[({[5-(dimethylamino) naphthalen-1yl]sulfinyl}oxy)amino]pentanoic acid and a squaraine dye, Moreover SDS and 2-naphtalenesulfonic acid (NSA), that can be used for dye dilution, were intercalated into LDH. LAG method was exploited to determine in short time if a number of molecules can be successfully intercalated into LDH. The tests performed on a quite large number of molecules allowed on one side to determine whether that particular molecule can be intercalated and on the other side to collect general data on the molecular features that favour the intercalation using Principal component analysis (PCA) and molecular descriptors to classify molecules. A total of about ten molecules were tested and 5 were successfully intercalated, while a partial intercalation was observed for some of them. These novel materials were characterized by X-ray powder diffraction and thermogravimetric analysis. To improve reaction yields, design of experiment (DOE) techniques were employed to find the optimal intercalation conditions for the partially successful cases and reach at least a 70-80% yield. Finally multivariate principal component analysis (PCA) was carried out to rationalize the success of the intercalation as a function of chemical descriptors, considering all the new molecules prepared by LAG method in current and in previous work (Conterosito et al. 2013 Cr Gr and des, 2013, *13* (3), 1162).