

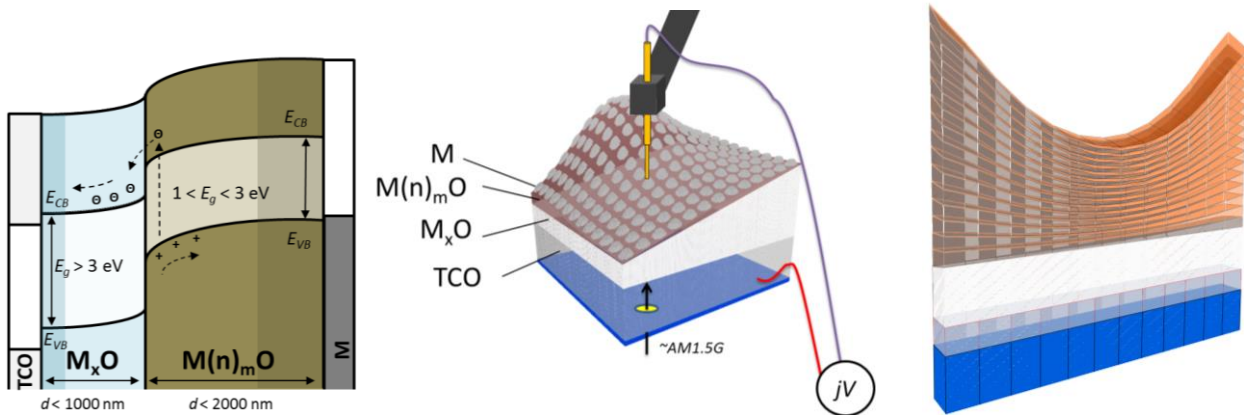
# Novel Absorbers for All Oxide Photovoltaics

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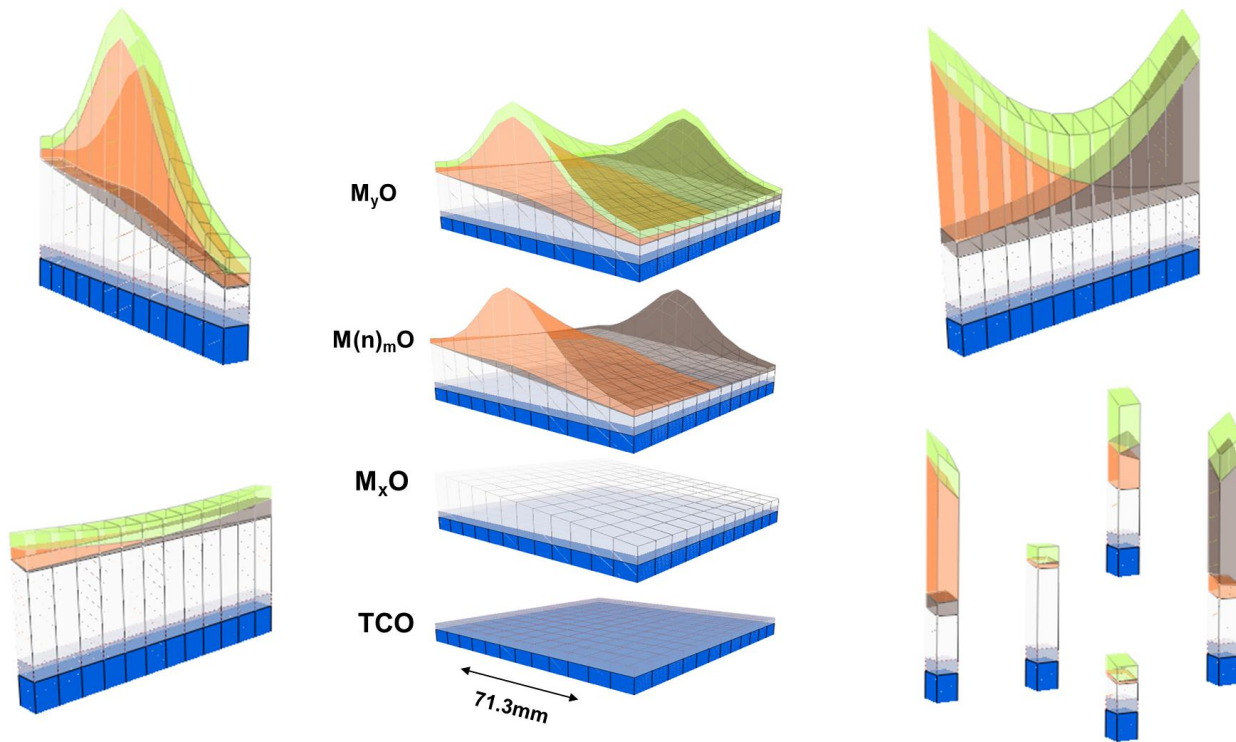
Owing to the past decade's demand for renewable energies, the PV market has shown great growth, facilitated by cost reductions<sup>1</sup> and the emergence of novel and promising technologies. Yet a significant gap between the ultimate PV platform and the currently available systems, calls for new PV technologies. Solar cells based on metal oxides have hardly been studied compared to other technologies, though photovoltaic effects surely exist in this type of semiconductor.<sup>2</sup> The abundance of metal oxides, combined with their low toxicity, ease of processing, low energy of processing, and stability can be considered ultimately as the basis for excellent photovoltaic modules.<sup>3</sup> Nevertheless, a metal oxide based solar cell that has high power conversion efficiency has not yet been realized. To achieve this goal, we perform a combinatorial materials study of metal oxide based light absorbers, charge transporters, junctions between them, and PV devices.



**Figure 1.** left - General schematic energy band diagram of a heterojunction all-oxide PV cell, approximated to form under short circuit conditions. M = Metal and O = Oxygen.  $M_xO$  is a window layer having a thickness,  $d$ , with the stoichiometric ratio  $x$ .  $M(n)_mO_x$  is a combinatorial light absorber material that can have  $n$  metals, each with the stoichiometric ratio  $m$  with respect to the oxygen. Stoichiometric variations in the light absorber cause changes in bandgap ( $E_g$ ), absorption coefficient, refractive index, charge carriers' type and concentration, excitons lifetime and allowed transitions. The fabrication parameters influence the thickness, morphology and crystallinity. The level of band bending, the position of the valence band edge ( $E_{vb}$ ), and the conduction band edge ( $E_{vb}$ ) of the

$M(n)_mO_x$  with respect to the  $M_xO$ , and the back contact metal (M) are approximations, more information can be found in <sup>4</sup>. **Center** - An example of a combinatorial library undergoes  $jV$  measurements under solar simulation. **Right** - a column of cells with a ternary combinatorial metal oxide absorber.

Figure 1 shows a schematic example of an energy band diagram and a basic working principle of a heterojunction all-oxide PV cell, formed between a wide bandgap semitransparent semiconductor, a layer of a combinatorial light absorber, metallic back contact and a transparent conducting oxide (TCO) as the front contact. Examples of elementary light absorbers are binaries of: Co–O, Cu–O, Mn–O or Fe–O, whereas  $TiO_2$ , ZnO,  $WO_3$  and NiO are examples of window layers (or selective contacts).



**Figure 2** –fabrication steps of a combinatorial device library (center). A single row, single columns and single cells (left and right) highlighting the different ratios between the window layer, light absorber and selective contact, as well as the ratio between doping or alloying of two oxides in a single absorber layer.

Doping, alloying or phase mixing between each of these oxides (wide or narrow bandgap), or with a non-conducting wide bandgap metal oxide (e.g. MgO, ZrO), or with metals, can provide novel ternaries, or a higher level of combinatorial materials, that can replace any of the layers shown in Figure 1.

The establishment of a solid combinatorial framework has already revealed novel materials and better device configurations with photovoltaic properties.<sup>5</sup> Further development of data mining and big data techniques, theoretical calculations and solidification of the current framework are expected to expedite the rate of discoveries and light on the current understanding of oxides in general.

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