# Benzoic Acid Surface Functionalization Of Conduction Band Engineered $Zn_{1-x}Mg_xO$ Layers For Enhanced Organic/Inorganic Photovoltaics

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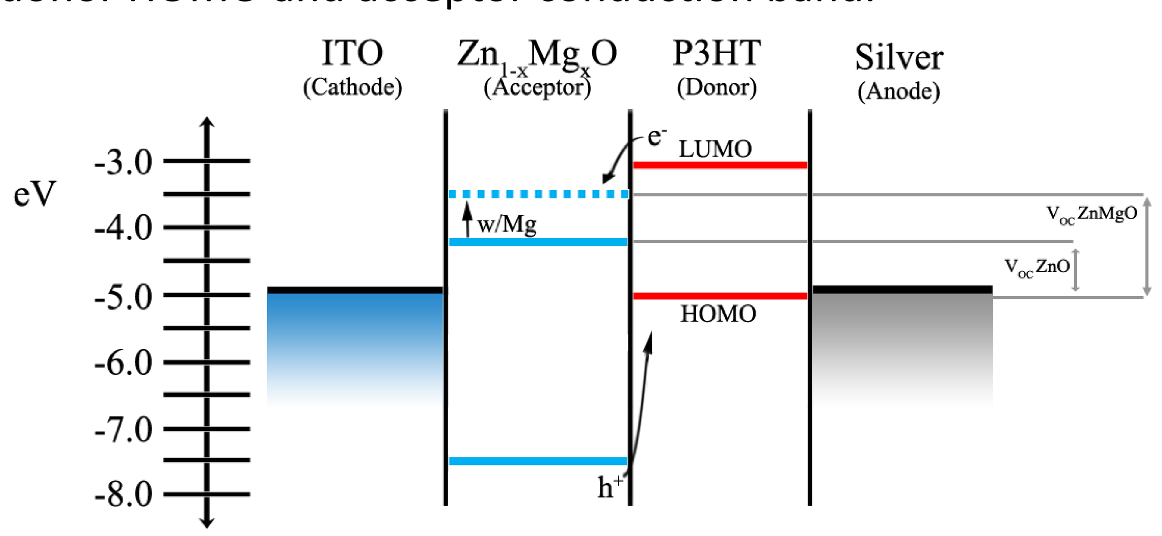
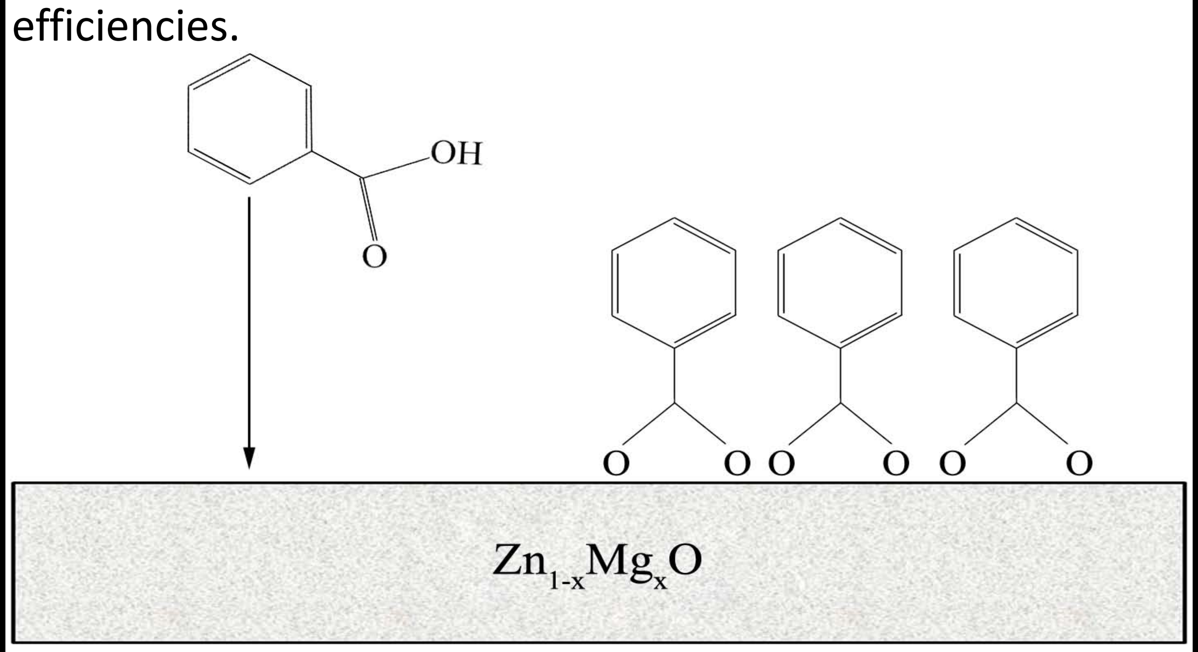
## Organic/Inorganic Photovoltaics 101

•Increasing the efficiency of organic/inorganic photovoltaics will open the door to a cheap, easy, and safe means to bring solar energy to the masses. A key role in raising this efficiency is by maximizing the band gap offset between donor HOMO and acceptor conduction band.




•Organic/inorganic photovoltaics are excitonic devices; they create an electric current by splitting an exciton produced in a donor layer whose electron is transferred from the donor to an acceptor, which then pushes the electron through to a conducting surface, producing a current. The efficiencies of these cells are extremely dependent upon the energy offset between the donor HOMO and acceptor conduction band – a larger offset ensures a higher $V_{OC}$ , which leads to higher efficiencies.




•One can perform conduction band tuning by alloying or introducing molecular dipoles to the surface. However, adsorbing these molecules to the surface often has negative effects, such as strong etching of the acceptor layer, ultimately rendering the device less effective.

## Our Goal

•Alloy ZnO with Mg to stifle the negative etching effects of acid adsorption, thereby retaining all the necessary absorption properties for electrical photoconversion.
•Study the bonding nature of carboxylic groups to the alloyed ZnO layer for refined preparative measures to produce the highest quality layers at the lowest cost .

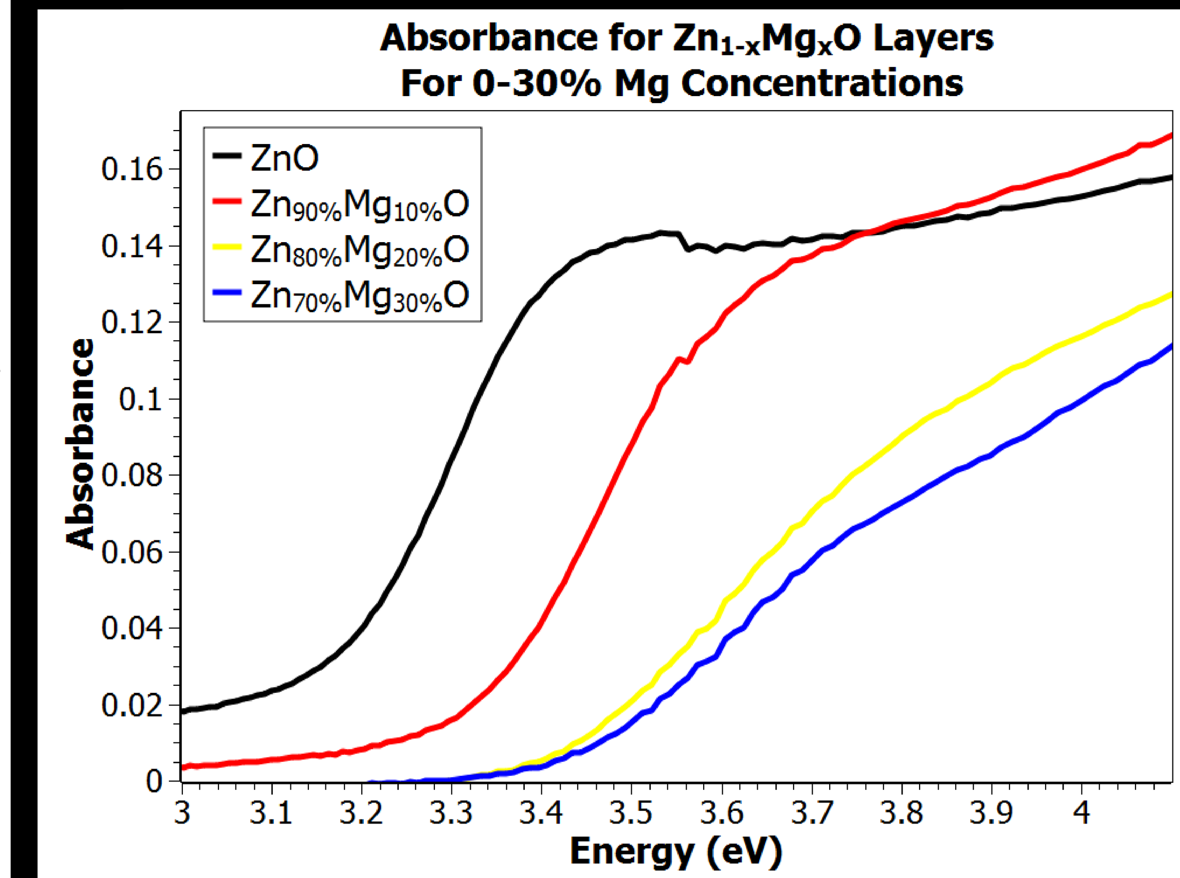
## Sample Preparation and Characterization

•Sol-gel samples were produced using a 5mL of 2-methoxy-ethanol and a 1:1 molar ratio of total metal acetate (zinc acetate-2-hydrate and magnesium acetate-4-hydrate) and ethanolamine. Solutions were stirred at 60°C @800 RPM for 30 minutes and spin coated onto a substrate for 60s @2000 RPM. The samples were then annealed according to the two following methods:

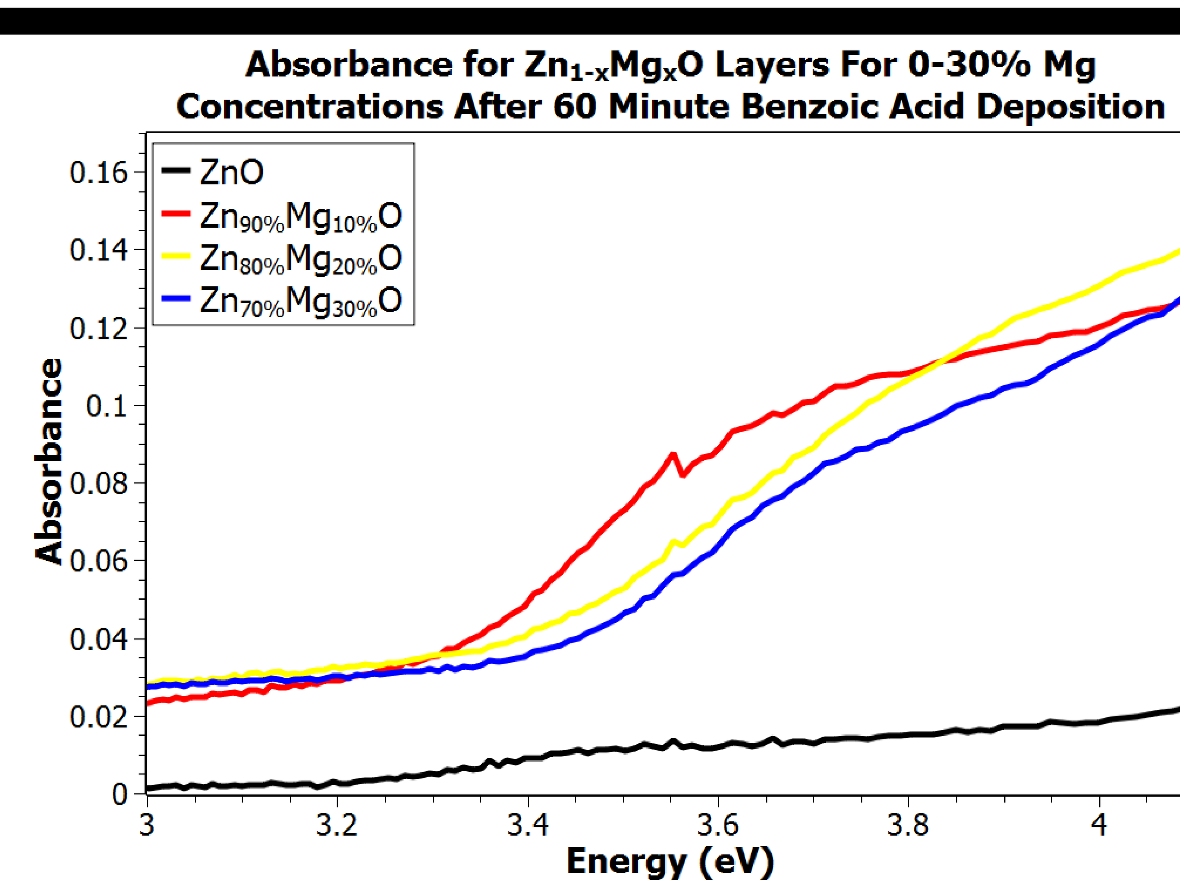
- •300°C for 5 minutes (Standard Approach)
- •200°C for 5 minutes, followed by 500°C for 5 minutes (Precursor Volatilization + Higher Crystallinity Approach, only where noted)

•Benzoic acid solution consisted of 2mM benzoic acid in hexane. Acid was deposited onto layers by soaking samples in acid solution for 60-240 minutes.

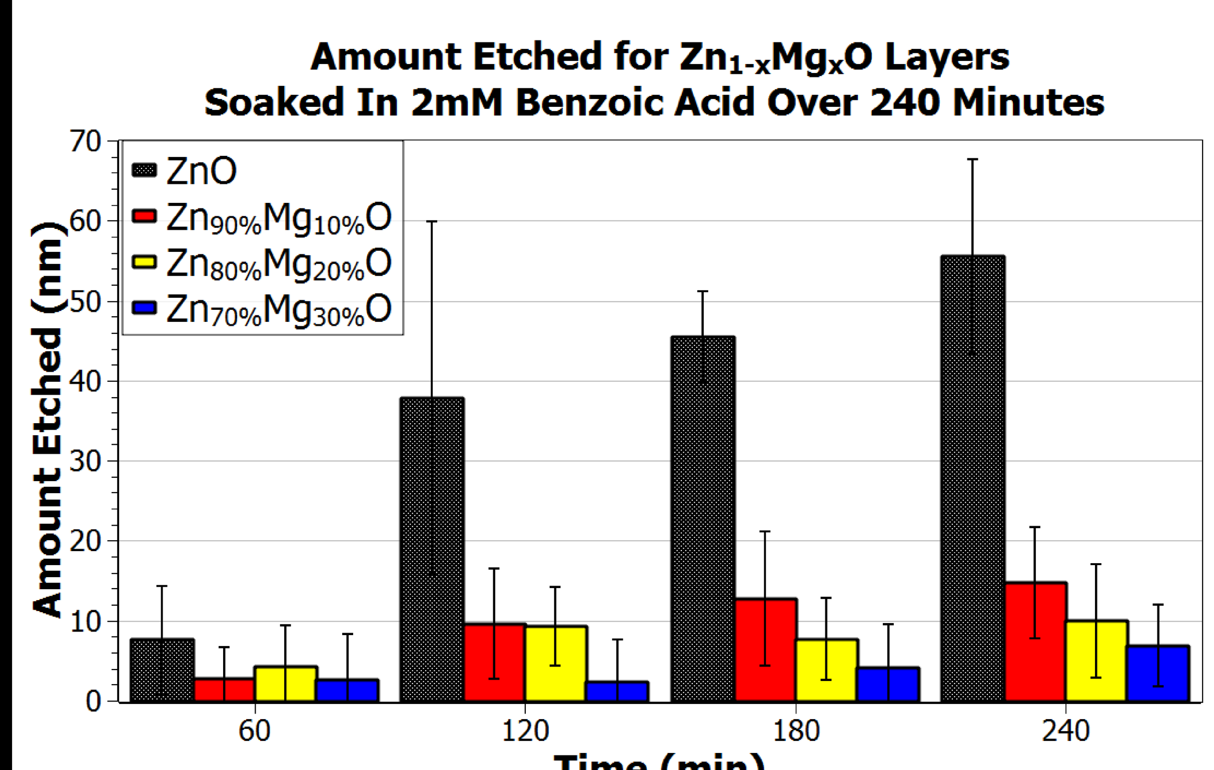
## Observed Tuning, Resistance to Etching, And Benzoic Acid Deposition



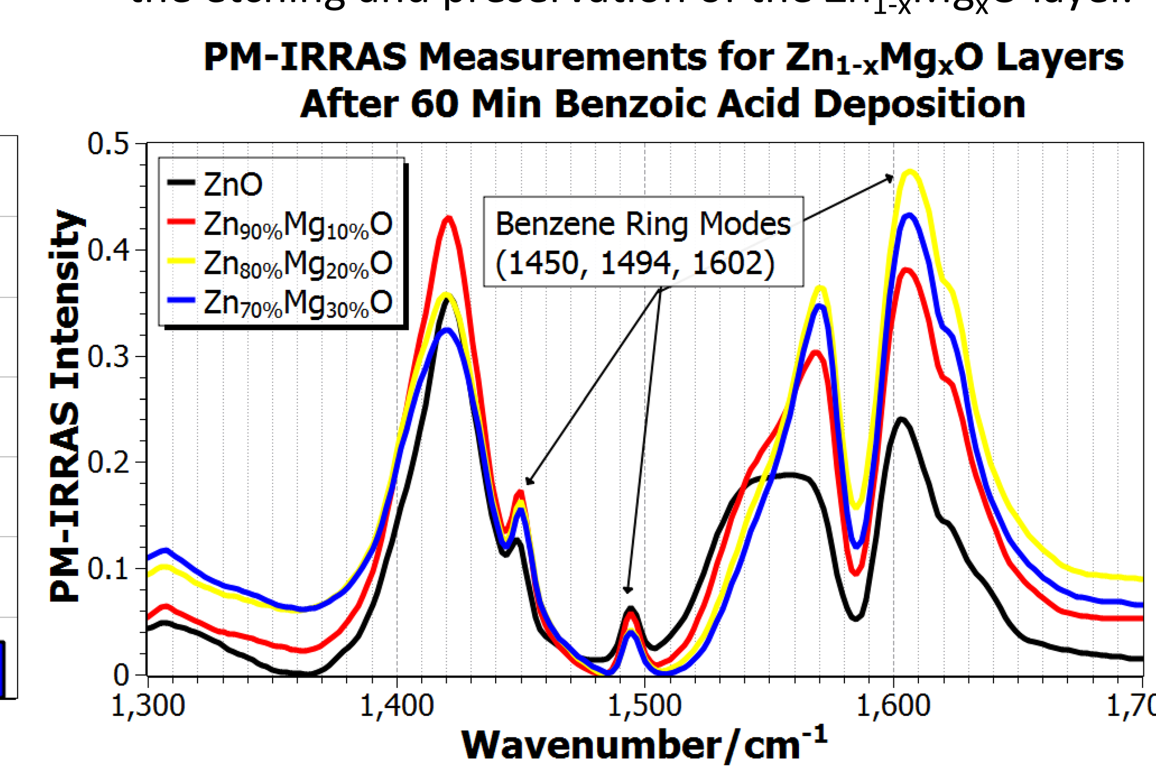

Alloying the ZnO layers with Mg shifts the absorbance signal to higher energies, signifying an increase in electronic band gap.




After adsorption of benzoic acid, a significant decrease in absorption can be seen in the layers of lower Mg concentration, while higher Mg concentrations preserve absorption. This is due to the etching and preservation of the $Zn_{1-x}Mg_xO$ layer.

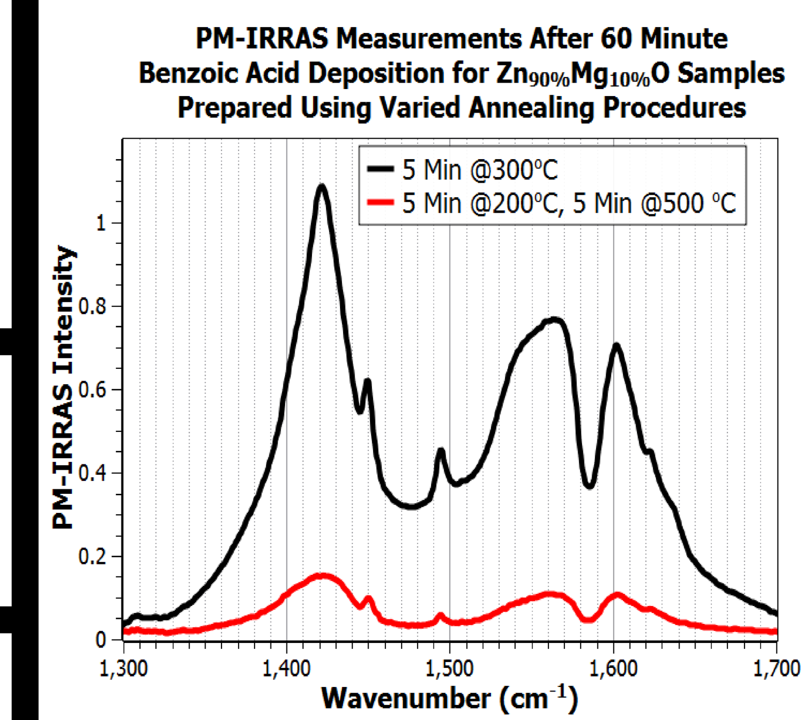



Profilometer measurements after acid adsorption indicate a much stronger etch resistance for $Zn_{1-x}Mg_xO$ layers with higher Mg concentration.

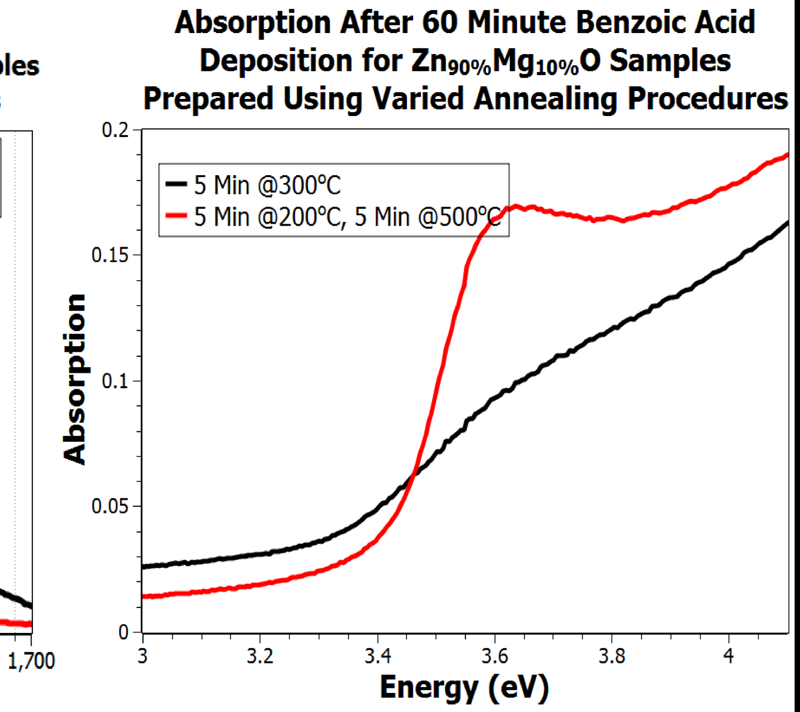



Vibrational benzene ring modes indicate adsorption of acid atop layers. Peaks at 1,421$cm^{-1}$ and 1,564$cm^{-1}$ indicate bonding to the surface.

## Eradication of Precursor and Enhanced Crystallinity




Alternative preparation method yields significantly less adsorbed material, signified by decreased ring and bond stretching modes.




Annealing at higher temperatures almost doubles the absorption for $Zn_{90\%}Mg_{10\%}O$ layers and increases etch resistance, indicating higher crystallinity.

## Conclusions and Future Work

•Observed direct relation between Mg concentration and resistivity to etching when in presence of benzoic acid.
•Successfully adsorbed benzoic acid to alloyed ZnO layers without ridding them entirely of their optoelectronic properties.
•Showed that current preparation methods may not be ideal, as eliminating the precursor and annealing at 500°C yields layers that are almost twice as effective at absorbing light energy at the band gap, as well as appearing to adsorb less benzoic acid.

•Etch resistance for Mg alloyed ZnO layers will give researchers an idea of how tuning the conduction band can simultaneously enhance their ability to functionalize the surface of the layer with any carboxylic acid by preventing the negative effects of acid adsorption.
•New annealing approach produces layers of higher crystallinity, which is more conducive to light energy absorption, as well as having strong effects as to how much acid adsorbs to the surface.

## Acknowledgements

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