

NETL CO₂ Capture Technology Meeting

Pacific

U.S. DEPARTMENT OF

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FST 1943

9 July 2012

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The U.S. DOE's Carbon Capture Simulation Initiative for Accelerating Commercialization of CCS Technology

- CCSI Toolset
- 5 Year Development Plan
- Technical Accomplishments
 - How these computational tools can be used today



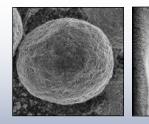


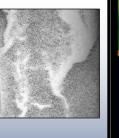






Carbon Capture Simulation Initiative











Identify promising concepts Reduce the time for design & 2 troubleshooting Quantify the technical risk, to enable reaching larger scales, earlier Stabilize the cost during commercial deployment



CCSI Timeline

- Organizational Meetings
 - March 2010 October 2010
- HQ organized Scientific Peer Review
 - January 25, 2011
- Technical work initiated
 - February 1, 2011
- Industry Advisory Board Workshops
 - February 2011
 - September 2011
 - April 2012
- Board of Directors Review
 - January 2012
- SCC Merit Review (ASME)
 - April 2012
- Preliminary Release of CCSI Toolset
 - September 2012

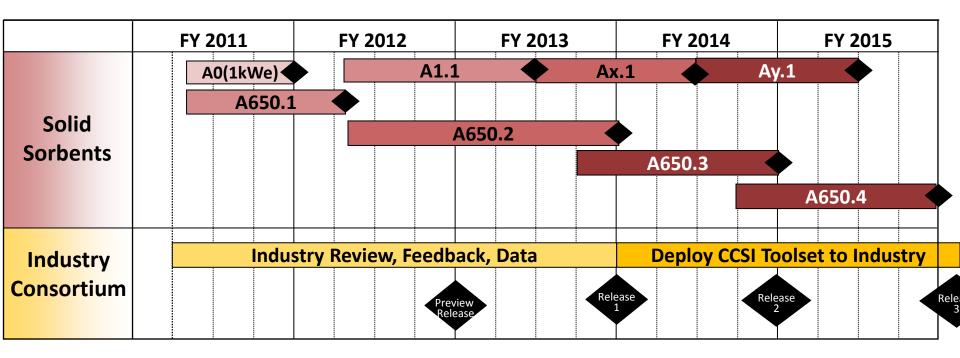








5 Year Plan for Demonstrating CCSI Toolset







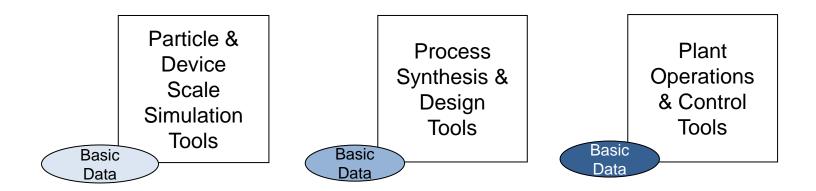








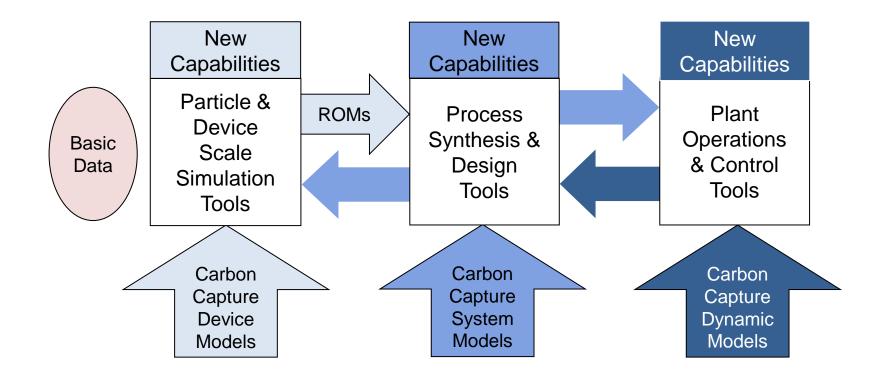
CCSI Toolset Overview







CCSI Toolset Overview





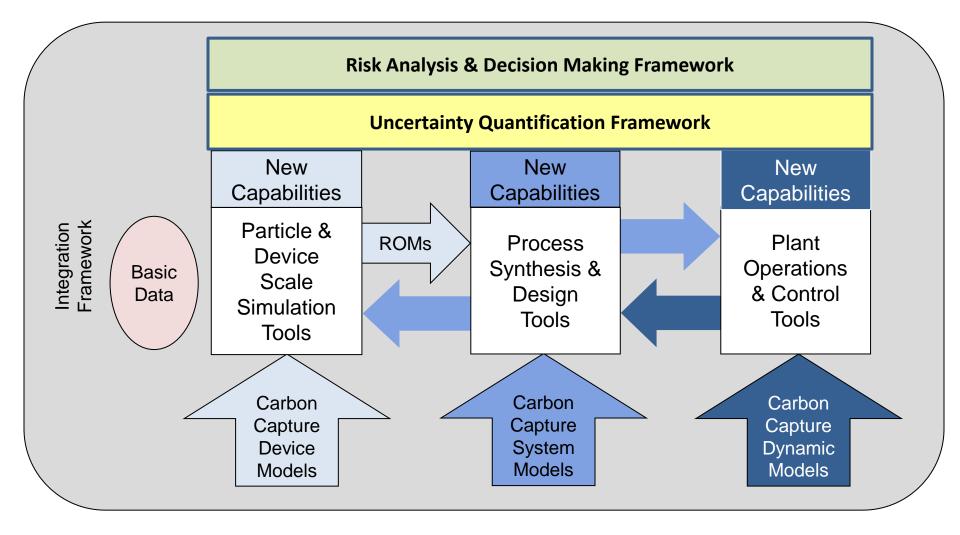








CCSI Toolset Overview





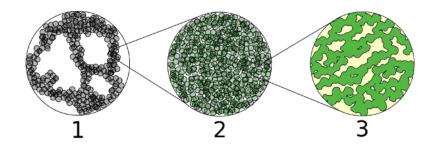


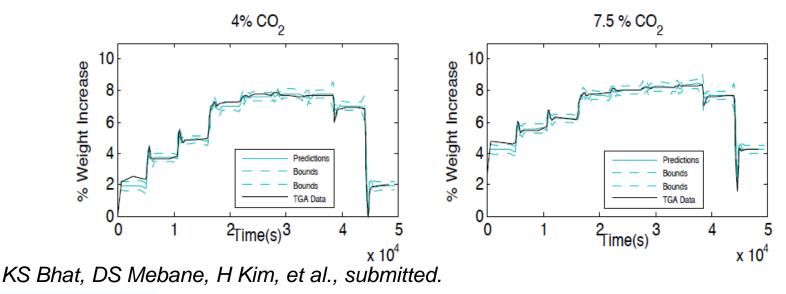


Sorbent Reaction Model with Bayesian-based UQ

- A general lumped kinetic model, quantitatively fit to TDA data, needed for initial CFD and process simulations
- High-fidelity model:
 - Sorbent microstructure broken down into three length scales
 - Separate treatment of gas-phase and polymer-phase transport
 - Accurately describes TGA features arising from bulk CO₂ transport effects

 $2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$ $R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$ $H_2O(gas) \rightleftharpoons H_2O(phys)$



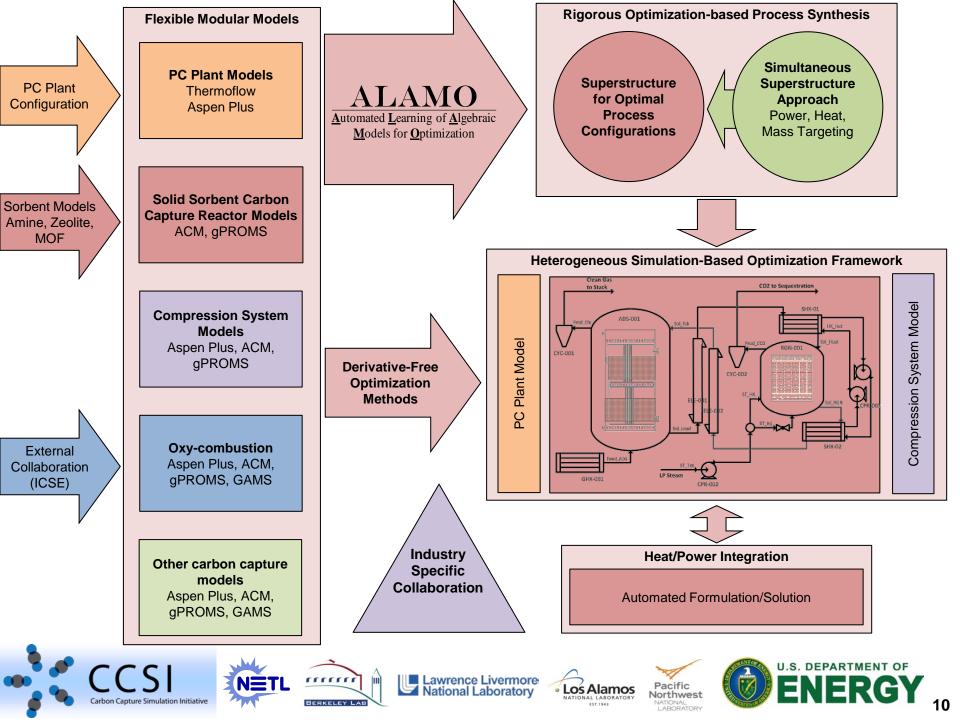


Lawrence Livermore

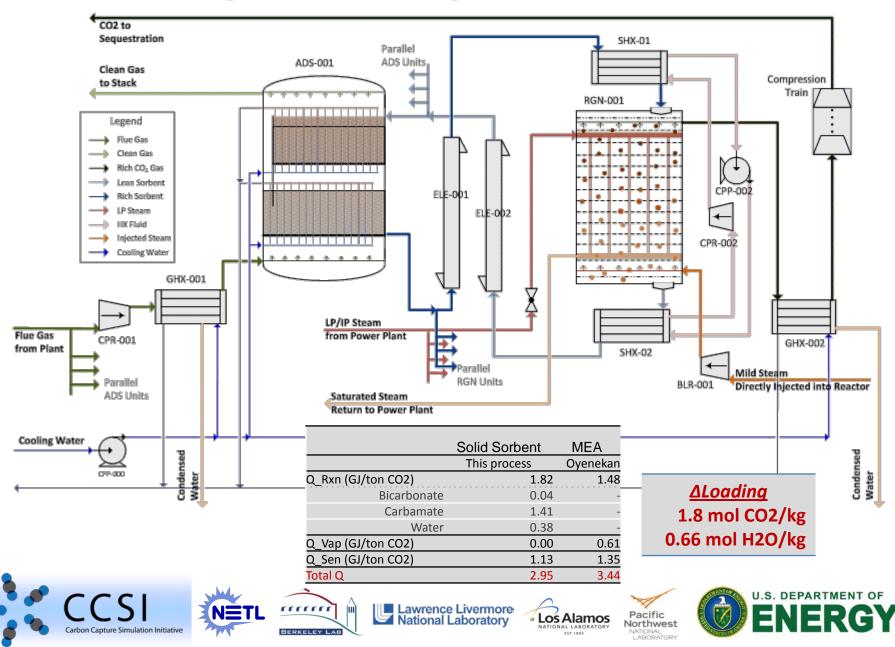
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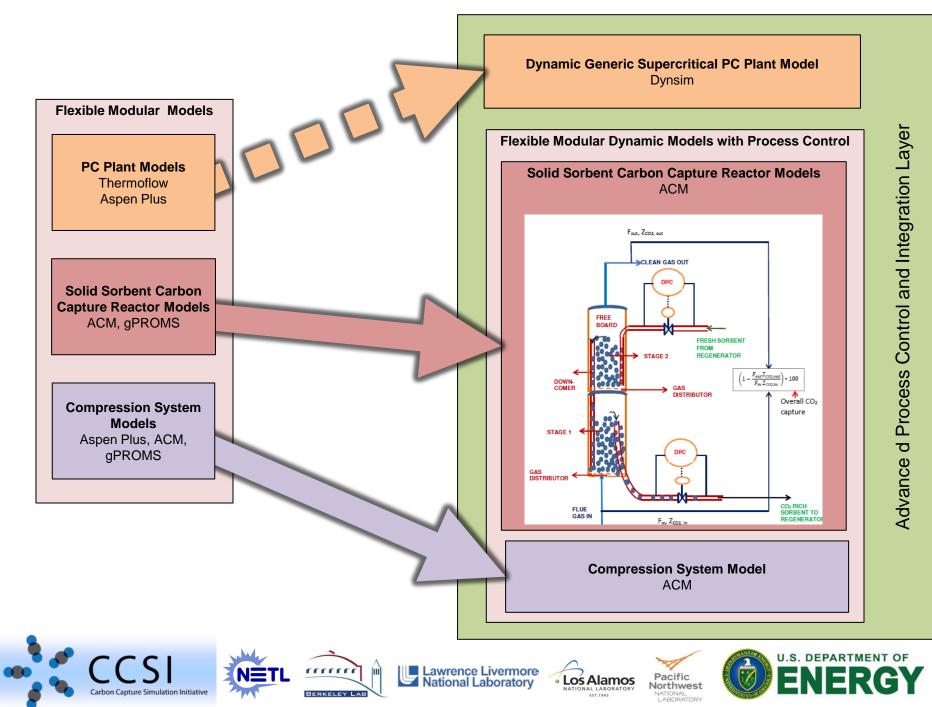




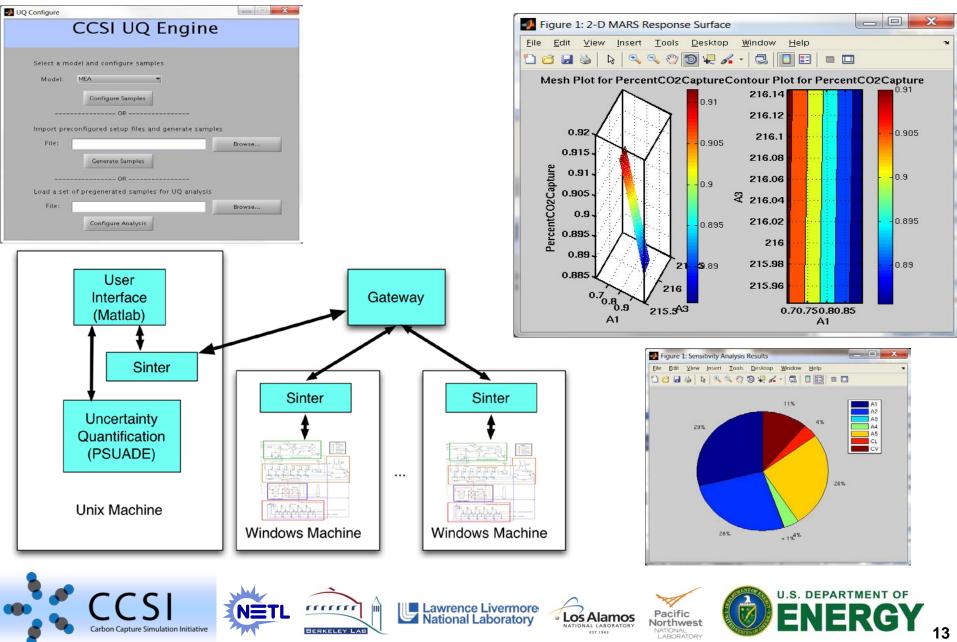
Optimized Capture Process



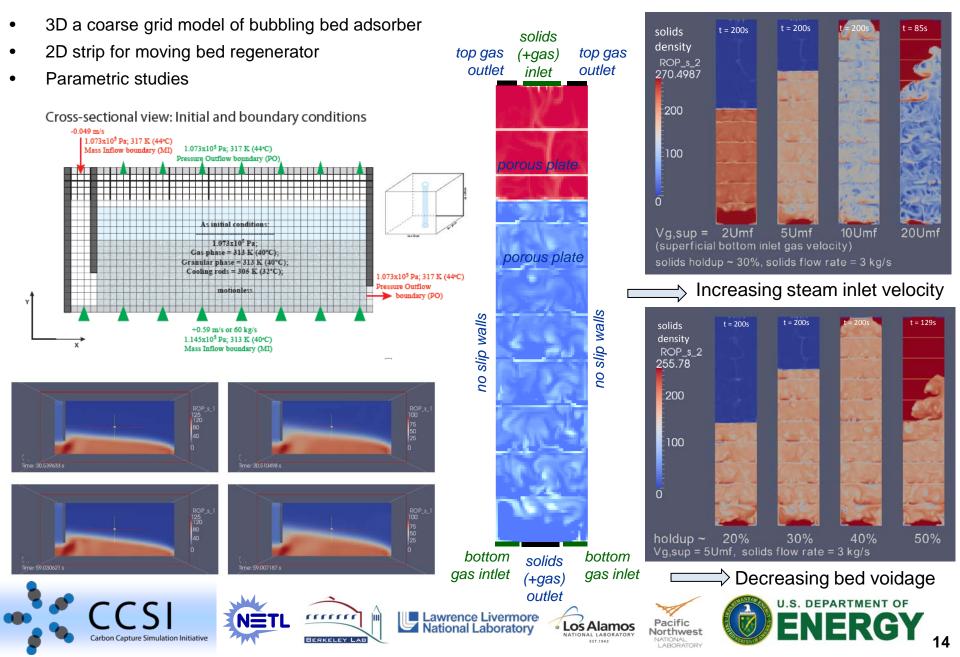
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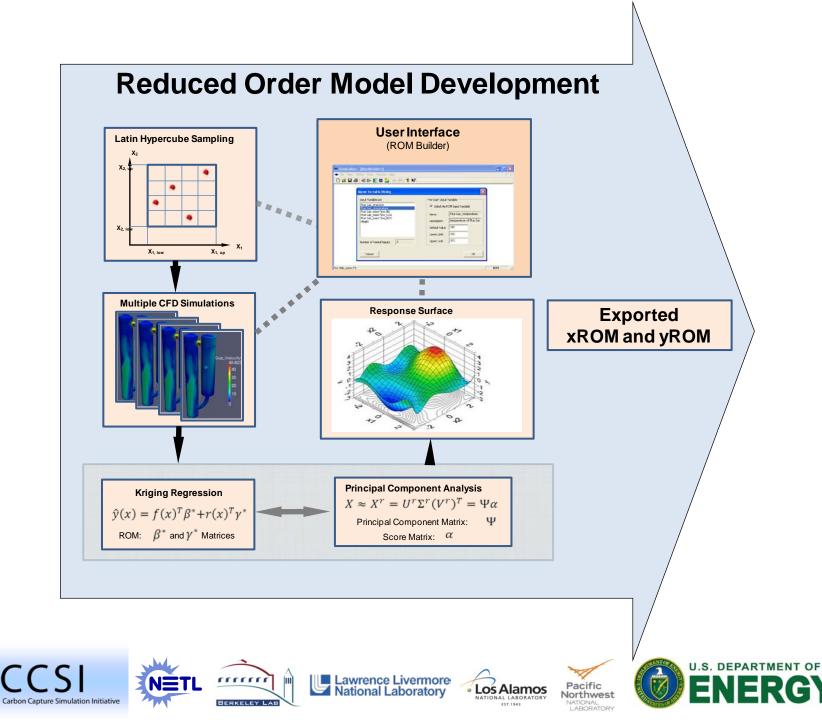


Link to Process Simulation for UQ Analysis

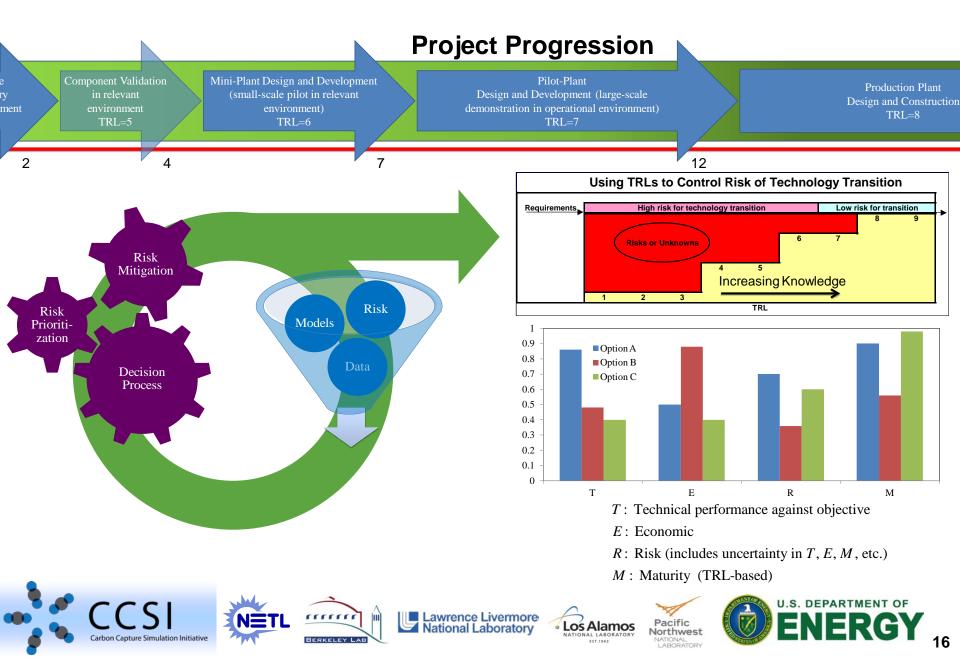


CFD of Adsorber & Regenerator (full scale, 1 MW)

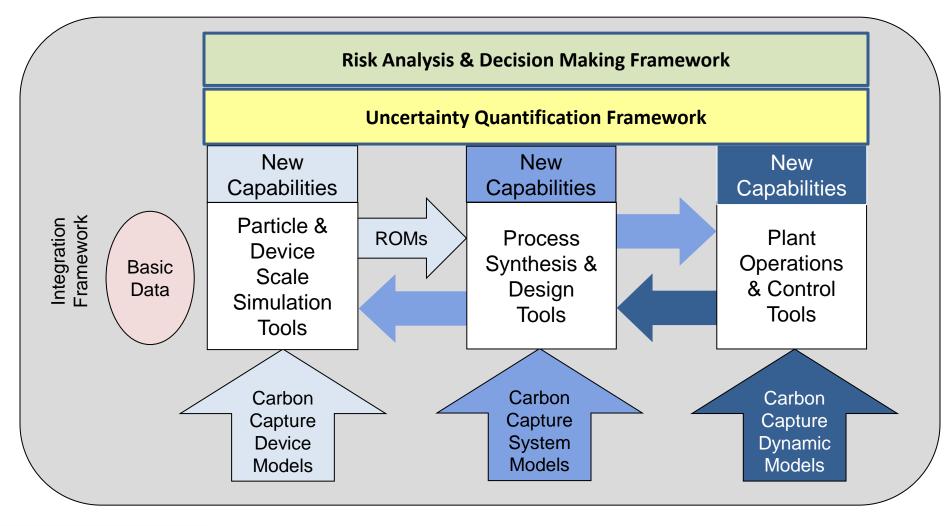




Formal Risk Metrics as Flexible Tools for Risk Analysis



Computational Tools to Accelerate Technology Development & Scale up



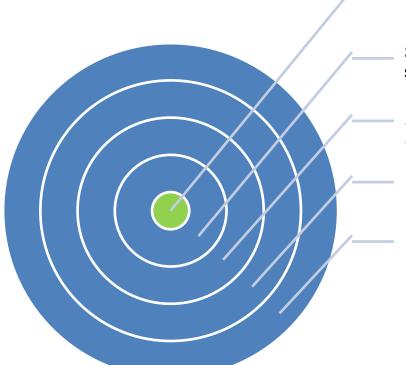








Potential Benefits to Program



Accelerate Commercialization of Carbon Capture Technology

Support decision making to move to largerscales, more quickly and with better designs

Use science-based models to assess and mitigate technical and financial risks, to improve designs, and to shorten the design cycle

Quantify uncertainties in the predictions of sciencebased models

Develop validated science-based models of carbon capture systems, integrating particle (droplet) and device scale models with process synthesis and design and process control













CCSI Collaboration Opportunities Roundtable - Woodlawn I

This evening @ 5 PM

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