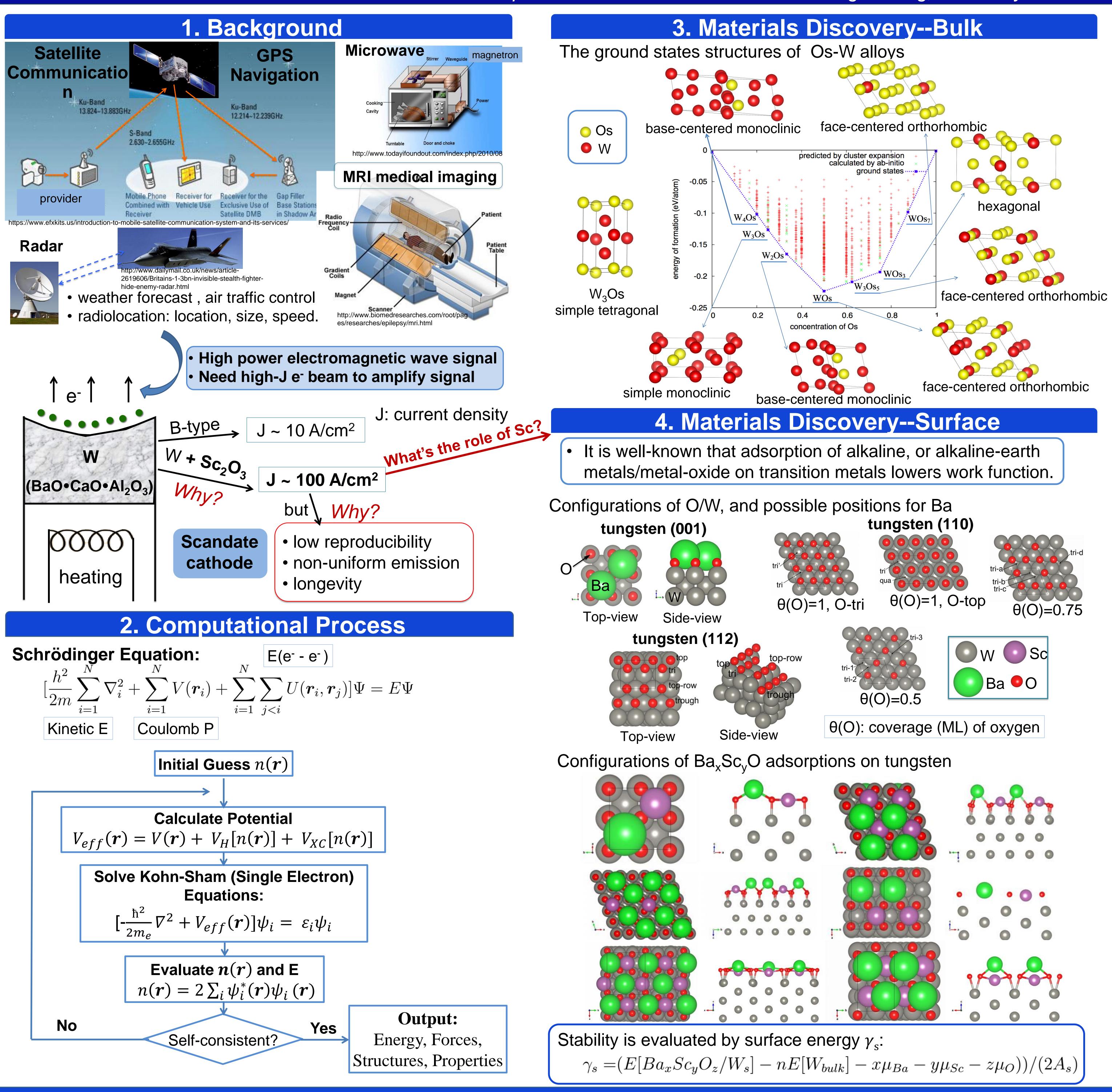
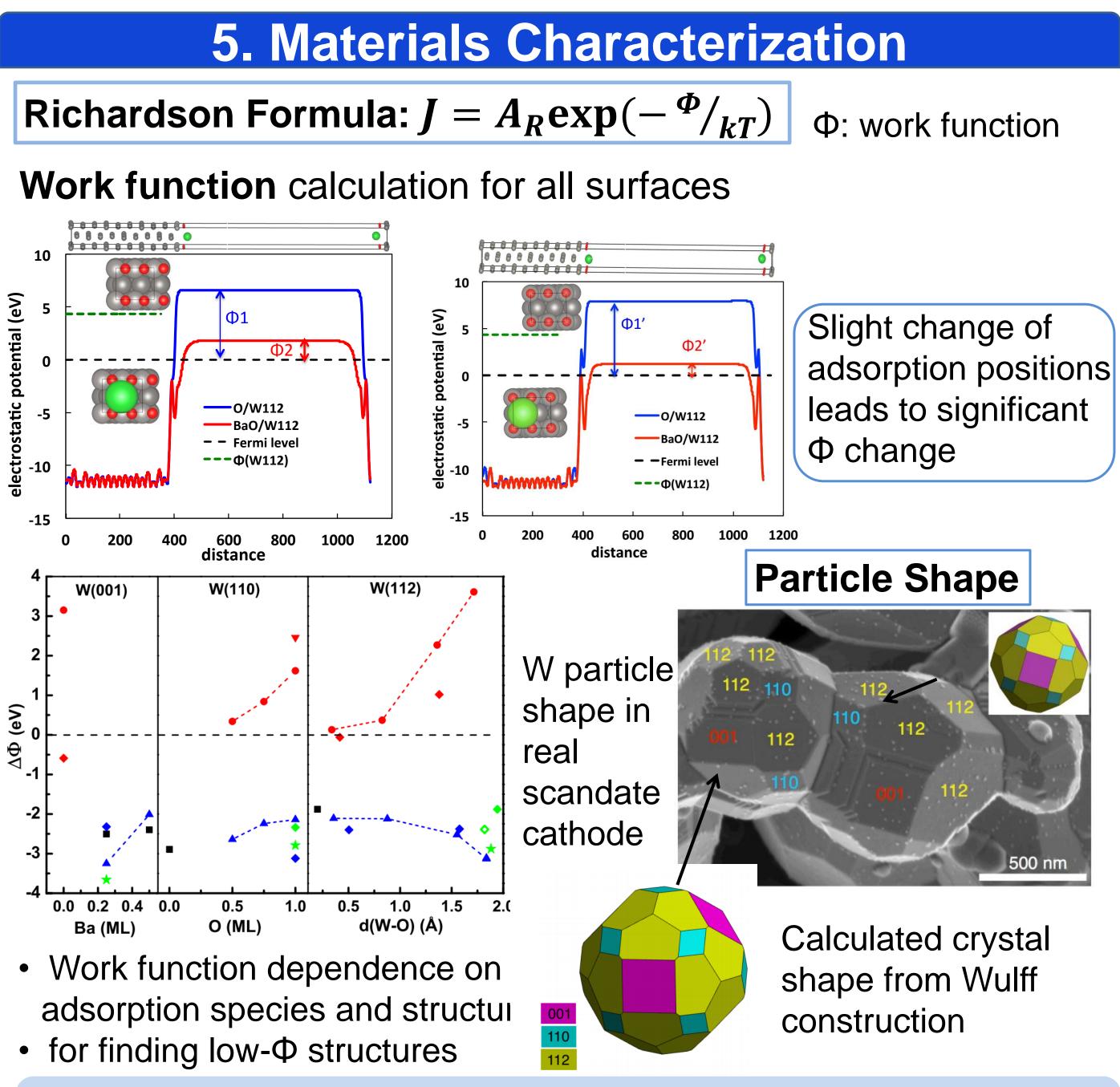
Computational Materials Characterization, Discovery, and Design with High **University of Kentucky** Performance Computing

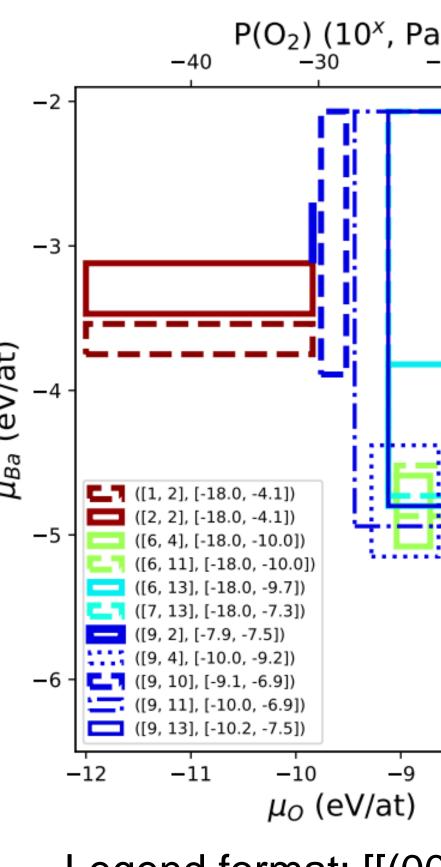


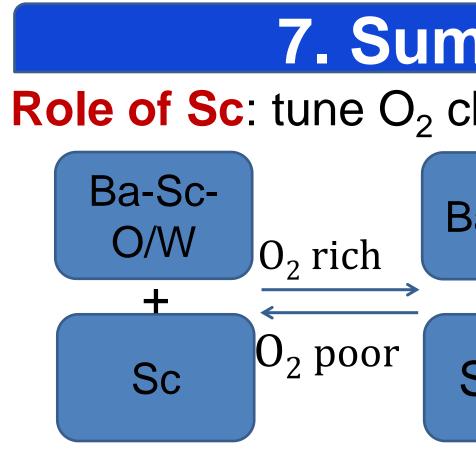
Qunfei Zhou, Xiaotao Liu, Tyler Maxwell, T. John Balk, and Matthew J. Beck Department of Chemical and Materials Engineering, University of Kentucky, Lexington, KY



With $\gamma_{(001)}$, $\gamma_{(110)}$, and $\gamma_{(112)}$ known, crystal shape can be calculated for every possible set of configurations.

6. Mate





erials a			($E[Ba_xSc$				$\left[k\right]$
-20 -10	1.8				_	$- z\mu_O))/(2$	-
	- 1.7	No.	(001) Str. bare Ba _{0.25}	Φ(eV) 4.48 1.98	No. 2 4	(112) Str. Ba _{0.5} O _{0.5} -row	Φ(eV) 1.75 5.35
	- 1.6	6 7 9	$\begin{array}{c} \text{Ba0.25O-top} \\ \text{Ba}_{0.5}\text{O-top} \\ \text{Ba}_{0.25}\text{Sc}_{0.25}\text{O} \end{array}$	1.23 2.47 0.82	10 11 13	$\begin{array}{c} Ba_{0.5}O_{0.5}\text{-row}\\ Ba_{0.5}O\text{-row}\\ Ba_{0.5}O\text{-top} \end{array}$	1.96 1.81 1.20
	- 1.5 () U	No.	(110) Str. bare Ba _{0.25}	Φ(eV) 4.81 1.92	(001) 1 2	all sets (112) 2 2	(110) 1 (1,2)
	- 1.4 Unctio - 1.3	3 4 5 9	O _{0.5} -tri O _{0.75} -tri O-tri Ba _{0.25} O-tri	5.15 5.65 6.43 2.67	(6,9) 6 (7,9) 9	$(4,11) \\ 13 \\ (11,13) \\ (2,10)$	(1,5,6) all but 2 all 2
	- 1.2 X - 1.2 X - 1.1 - 1.0	9 Ba _{0.25} O-tri 2.67 9 (2,10) 2 Ranges of μ_{Ba} , μ_0 , and μ_{Sc} where sets of configurations: • Stable • Have very low Φ ; • Yield right crystal shape;					

Legend format: [[(001), (112)], [min(μ_{Sc}), max(μ_{Sc})]]

7. Summary and Future Work

chemical potential Future work:					
Ba-O/W	 Further experiments to verify the computational work; 				
+	 Fabricate improved cathodes by 				
Sc ₂ O ₃	tuning: μ_{Ba} : >-5.0 eV μ_0 : -7.4 eV ~ -9.5 eV				

f.z@uky.edu