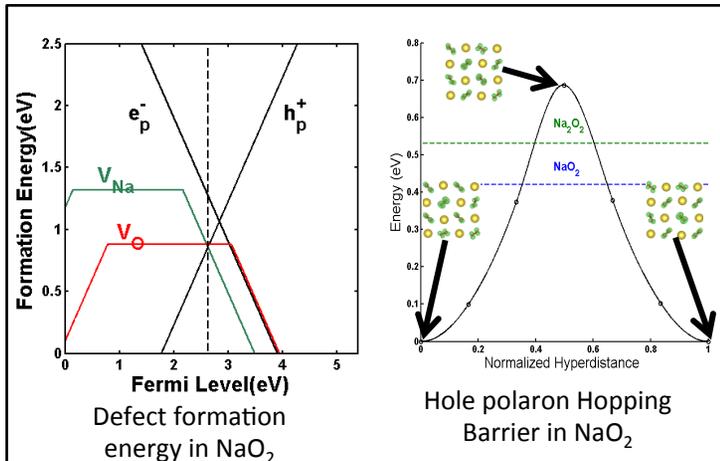




Does Enhanced Conductivity Lead to Low Charging Overpotentials in NaO_2 ?



Left: Formation energies of O vacancies (red lines), Na vacancies (green lines), electron polarons and hole polarons (black lines). Positively-charged defects have a positive slope while negative defects have a negative slope.

Right: Preliminary hopping pathways (single-point energies only) for hole polarons in NaO_2 . Ball-and-stick models with magnetization density isosurfaces (green) are shown for the intralayer hopping between nearest neighbor O-O dimers in NaO_2 .

Scientific Achievement

Predicted charge carrier concentrations and mobilities in bulk Na_2O_2 and NaO_2 by combining quasi-particle GW methods, hybrid-functional based DFT calculations, and transition state theory.

Significance and Impact

Suggests that the high efficiency (low-charge overpotentials) observed in Na-air batteries does not arise from high bulk conductivity in NaO_2 .

Research Details

- Hole polarons and negative sodium vacancies are the dominant charge-carrying defects in both Na_2O_2 and NaO_2 .
- Based on calculated carrier concentrations and preliminary data for the mobilities, the conductivities of Li_2O_2 , Na_2O_2 and NaO_2 are expected to be similar, and low overall. Further calculations to refine the polaron hopping barrier in NaO_2 are in progress.
- The comparable conductivities for Na_2O_2 and NaO_2 suggest that enhanced bulk charge transport is *not responsible* for lower charging overpotentials in Na-air cells that discharge to NaO_2 .



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High-level Performance Metrics

- Joint conferences, workshops and symposia organized
 - 4 CERC-CVC-wide meetings, 9 EVI workshops
 - >100 Technical meetings (mostly by individual TA)
- Journal and conference papers published
 - >292 papers published or accepted
- IP disclosures filed; US, China, and international patents issued
 - 30 in China, 28 in US (17 from Chinese side)
- Number, frequency, duration of personnel exchanged/collocated among organizations
 - ~ 100 short-term visits, 25 long-term (> 30 days) visits planned or executed



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Thank You!



Chengdu Panda Base
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