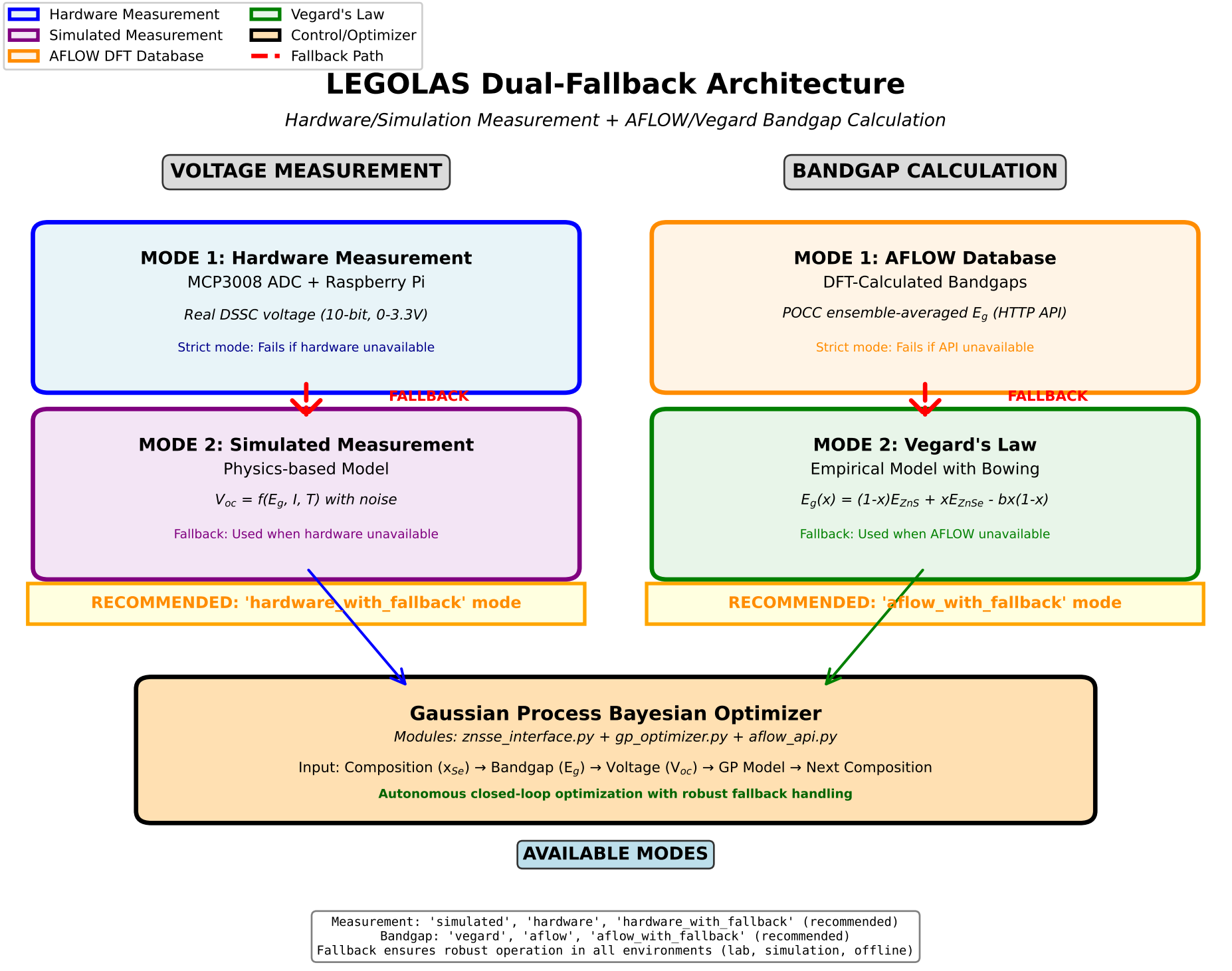
Hardware Measurement
Simulated Measurement
AFLOW DFT Database
Vegard's Law
Control/Optimizer
Fallback Path
LEGOLAS Dual-Fallback Architecture
Hardware/Simulation Measurement + AFLOW/Vegard Bandgap Calculation
VOLTAGE MEASUREMENT
BANDGAP CALCULATION
MODE 1: Hardware Measurement
MCP3008 ADC + Raspberry Pi
Real DSSC voltage (10-bit, 0-3.3V)
Strict mode: Fails if hardware unavailable
FALLBACK
MODE 2: Simulated Measurement
Physics-based Model
$V_{oc} = f(E_g, I, T)$ with noise
Fallback: Used when hardware unavailable
RECOMMENDED: 'hardware_with_fallback' mode
MODE 1: AFLOW Database
DFT-Calculated Bandgaps
POCC ensemble-averaged E_g (HTTP API)
Strict mode: Fails if API unavailable
FALLBACK
MODE 2: Vegard's Law
Empirical Model with Bowing
$E_g(x) = (1-x)E_{ZnS} + xE_{ZnSe} - bx(1-x)$
Fallback: Used when AFLOW unavailable
RECOMMENDED: 'aflow_with_fallback' mode
Gaussian Process Bayesian Optimizer
Modules: znsse_interface.py + gp_optimizer.py + aflow_api.py
Input: Composition (x_{Se}) → Bandgap (E_g) → Voltage (V_{oc}) → GP Model → Next Composition
Autonomous closed-loop optimization with robust fallback handling
AVAILABLE MODES
Measurement: 'simulated', 'hardware', 'hardware_with_fallback' (recommended)
Bandgap: 'vegard', 'aflow', 'aflow_with_fallback' (recommended)
Fallback ensures robust operation in all environments (lab, simulation, offline)