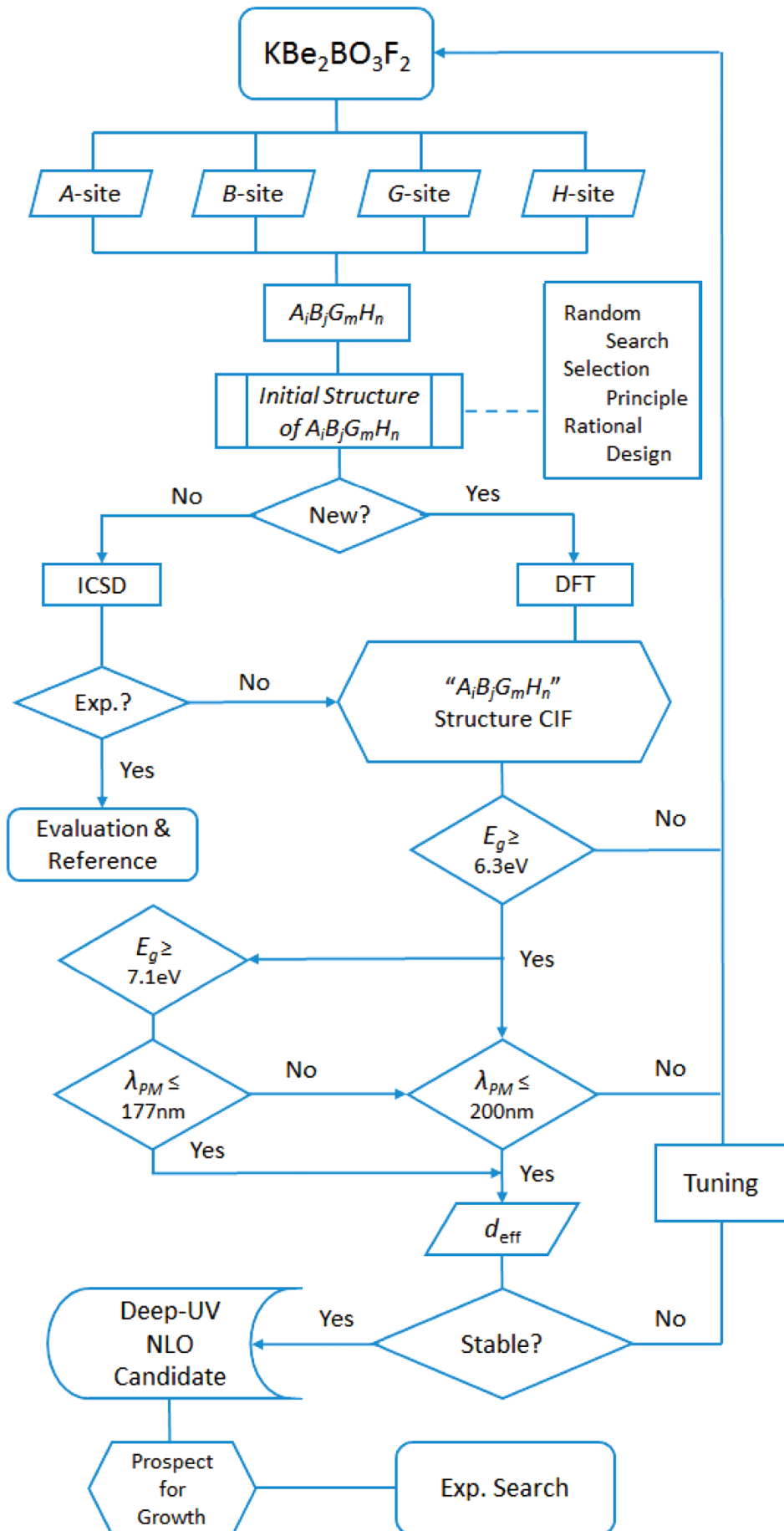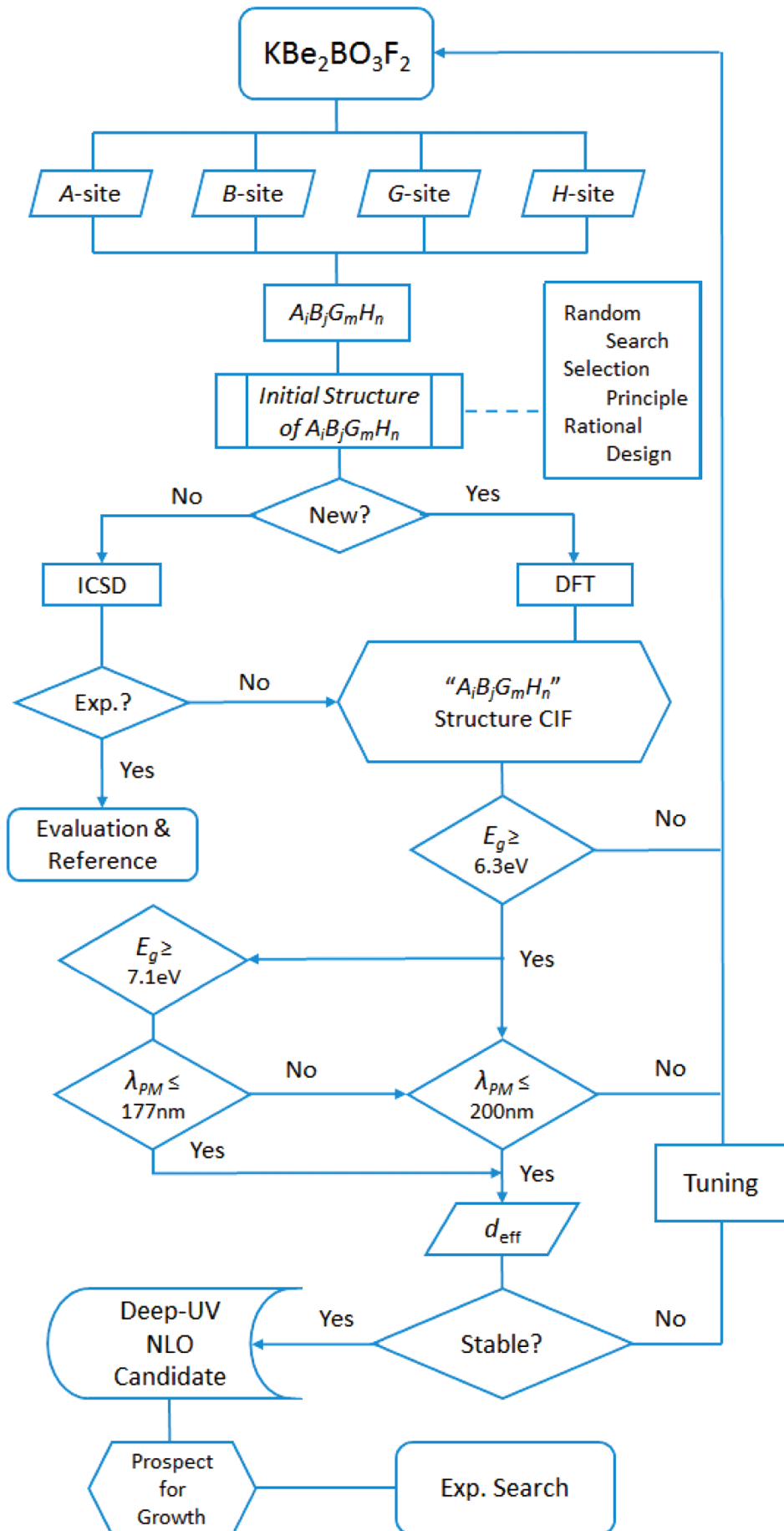[X Force Keygen Advance Steel 2019](#)

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$KBe_2BO_3F_2$

A-site B-site G-site H-site

$A_iB_jG_mH_n$

Random Search Selection Principle Rational Design

Initial Structure of $A_iB_jG_mH_n$

New?

No — ICSD

Yes — DFT

Exp.?

No → "$A_iB_jG_mH_n$" Structure CIF

Yes → Evaluation & Reference

$E_g \geq 6.3eV$

No

$E_g \geq 7.1eV$

Yes

$\lambda_{PM} \leq 177nm$

No

$\lambda_{PM} \leq 200nm$

No

Yes

Yes

Tuning

d_{eff}

Stable?

Yes → Deep-UV NLO Candidate

No

Prospect for Growth — Exp. Search

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